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<p>(51) International Patent Classification 7 : A61K 31/505, C07D 401/14, 413/14, 417/12, 405/12, 401/12</p>	<p>A1</p>	<p>(11) International Publication Number: WO 00/47212 (43) International Publication Date: 17 August 2000 (17.08.00)</p>
<p>(21) International Application Number: PCT/GB00/00373 (22) International Filing Date: 8 February 2000 (08.02.00) (30) Priority Data: 99400305.1 10 February 1999 (10.02.99) EP (71) Applicants (for all designated States except US): AS-TRAZENECA UK LIMITED [GB/GB]; 15 Stanhope Gate, London W1Y 6LN (GB); ZENCA-PHARMA S.A. [FR/FR]; Le Galien, 1, rue des Chauffours, Boite postale 127, F-95022 Cergy Cedex (FR). (72) Inventors; and (75) Inventors/Applicants (for US only): HENNEQUIN, Laurent, François, Andre [FR/FR]; Z.I. La Pompelle, Boite postale 1050, F-51689 Reims Cedex 2 (FR); PLE, Patrick [FR/FR]; Z.I. La Pompelle, Boite postale 1050, F-51689 Reims Cedex 2 (FR); STOKES, Elaine, Sophie, Elizabeth [GB/GB]; Alderley Park, Macclesfield, Cheshire SK10 4TG (GB); MCKERRECHER, Darren [GB/GB]; Alderley Park, Macclesfield, Cheshire SK10 4TG (GB). (74) Agent: BRYANT, Tracey; AstraZeneca, Global Intellectual Property, Patents, Mereside, Alderley Park, Macclesfield, Cheshire SK10 4TG (GB).</p>		<p>(81) Designated States: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).</p> <p>Published With international search report.</p>
<p>(54) Title: QUINAZOLINE DERIVATIVES AS ANGIOGENESIS INHIBITORS</p> <div data-bbox="455 877 677 1005" data-label="Chemical-Block"> </div> <p>(57) Abstract</p> <p>The invention relates to the use of compounds of formula (I), wherein ring C is an 8, 9, 10, 12 or 13-membered bicyclic or tricyclic moiety which optionally may contain 1-3 heteroatoms selected independently from O, N and S; Z is -O-, -NH-, -S-, -CH₂- or a direct bond; n is 0-5; m is 0-3; R² represents hydrogen, hydroxy, halogeno, cyano, nitro, trifluoromethyl, C₁-alkyl, C₁-alkoxy, C₁-alkylsulphonyl, -NR³R⁴ (wherein R³ and R⁴, which may be the same or different, each represents hydrogen or C₁-alkyl), or R⁵X¹ (wherein X¹ and R⁵ are as defined herein; R¹ represents hydrogen, oxo, halogeno, hydroxy, C₁-alkoxy, C₁-alkyl, C₁-alkoxymethyl, C₁-alkanoyl, C₁-phaloalkyl, cyano, amino, C₂-alkenyl, C₂-alkynyl, C₁-alkanoyloxy, nitro, C₁-alkanoylamino, C₁-alkoxycarbonyl, C₁-alkylsulphonyl, C₁-alkylsulphonyl, C₁-alkylsulphonyl, carbamoyl, N-C₁-alkylcarbamoyl, N,N-di(C₁-alkyl)carbamoyl, aminosulphonyl, N-C₁-alkylaminosulphonyl, N,N-di(C₁-alkyl)aminosulphonyl, N-(C₁-alkylsulphonyl)amino, N-(C₁-alkylsulphonyl)-N-(C₁-alkyl)amino, N,N-di(C₁-alkylsulphonyl)amino, a C₂-alkylene chain joined to two ring C carbon atoms, C₁-alkanoylamino-C₁-alkyl, carboxy or a group R⁶X¹⁰ (wherein X¹⁰ and R⁶ are as defined herein); and salts thereof, in the manufacture of a medicament for use in the production of an antiangiogenic and/or vascular permeability reducing effect in warm-blooded animals, processes for the preparation of such compounds, pharmaceutical compositions containing a compound of formula (I) or a pharmaceutically acceptable salt thereof as active ingredient and compounds of formula (I). The compounds of formula (I) and the pharmaceutically acceptable salts thereof inhibit the effects of VEGF, a property of value in the treatment of a number of disease states including cancer and rheumatoid arthritis.</p>		

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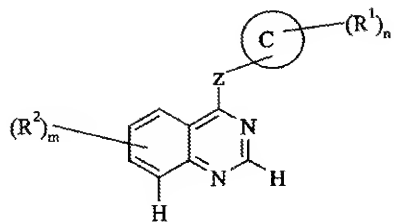
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(54)【発明の名称】 血管形成阻害剤としてのキナゾリン誘導体

(57)【要約】

本発明は、式 I の化合物 [式 C、環 C は、O、N 及び S から独立して選択される 1~3 個のヘテロ原子を場合に
 より含有し得る 8、9、10、12 又は 13 員の二環式
 又は三環式部分であり；Z は -O-、-NH-、-S-
 -、-CH₂-又は直接の結合であり；n は 0~5 の整
 数であり；m は 0~3 の整数であり；R²は水素、ヒド
 ロキシ、ハロゲン、シアノ、ニトロ、トリフルオロメチ
 ル、C₁₋₃アルキル、C₁₋₃アルコキシ、C₁₋₃アルキル
 スルファニル、-NR³R⁴ (ここで、R³及びR⁴は同じ
 であっても異なってもよく、それぞれ水素又は C₁₋₃
 アルキルを表す)、又は R⁵X¹⁰を表し (ここで、
 X¹及びR⁵は本明細書に定義される通りである)；R¹
 は水素、オキソ、ハロゲン、ヒドロキシ、C₁₋₄アルコ
 キシ、C₁₋₄アルキル、C₁₋₄アルコキシメチル、C₁₋₄
 アルカノイル、C₁₋₄ハロアルキル、シアノ、アミノ、
 C₂₋₆アルケニル、C₂₋₆アルキニル、C₁₋₃アルカノイ
 ルオキシ、ニトロ、C₁₋₄アルカノイルアミノ、C₁₋₄アル
 コキシカルボニル、C₁₋₄アルキルスルファニル、C₁₋₄
 アルキルスルフィニル、C₁₋₄アルキルスルホニル、

カルバモイル、N-C₁₋₄アルキルカルバモイル、N、
 N-ジ (C₁₋₄アルキル) カルバモイル、アミノスルホ
 ニル、N-C₁₋₄アルキルアミノスルホニル、N、N-
 ジ (C₁₋₄アルキル) アミノスルホニル、N- (C₁₋₄アル
 キルスルホニル) アミノ、N- (C₁₋₄アルキルスル
 ホニル) -N- (C₁₋₄アルキル) アミノ、N、N-ジ
 (C₁₋₄アルキルスルホニル) アミノ、環 C の 2 つの炭
 素原子に結合した C₃₋₇アルキレン鎖、C₁₋₄アルカノイ
 ルアミノ C₁₋₄アルキル、カルボキシ、又は R⁵X¹⁰を
 表す (ここで、X¹⁰及びR⁵は本明細書に定義される通
 りである)、及びその塩の、温血動物において抗血管
 形成効果及び/又は血管透過性抑制効果を生ずるのに使
 用する医薬品の製造における使用、そのような化合物の
 製造法、式 (I) の化合物又はその製剤的に許容される
 塩を有効成分として含有する医薬組成物、及び式 (I)
 の化合物群に関する。式 (I) の化合物及びその製剤的
 に許容される塩は VEGF の作用を阻害し、これは癌及
 び慢性閉塞性肺病を含む数多くの病態の治療において
 有用な特性である。



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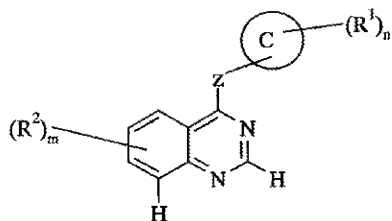
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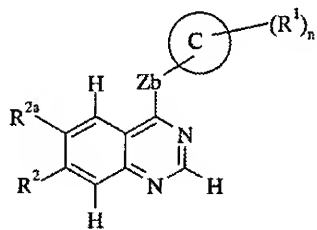
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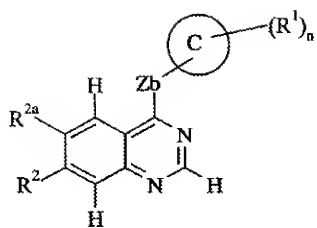
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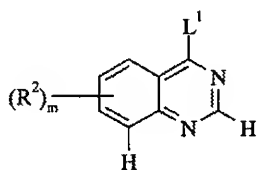
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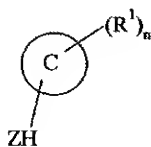
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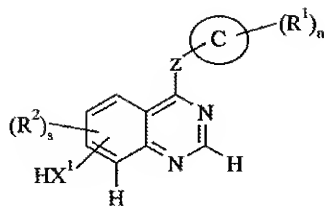
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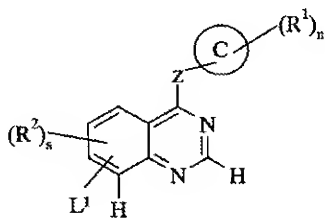
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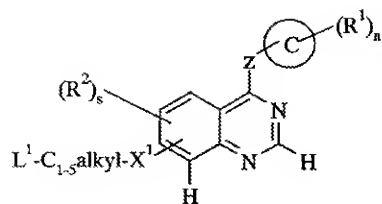


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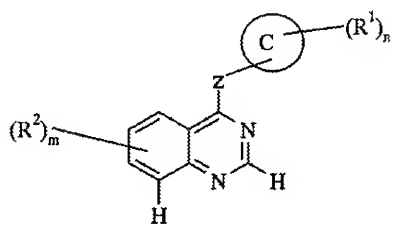
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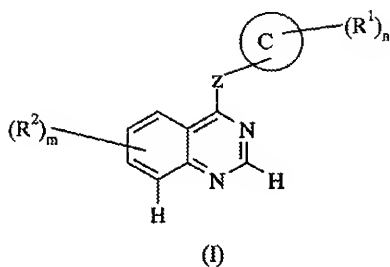
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This image shows a full page of white paper with horizontal dotted lines. The lines are evenly spaced and run across the width of the page, providing a guide for handwriting practice. There are no margins, text, or other markings on the page.

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This image shows a full page of a document template designed for handwritten notes or answers. It features approximately 28 evenly spaced horizontal rows of small dots, providing a guide for letter height and placement. The entire page is otherwise blank, with no margins, headers, or footers visible.

This image shows a full page of white paper with horizontal dotted lines. The lines are evenly spaced and run across the width of the page, providing a guide for handwriting practice. There are no margins, text, or other markings on the page.

[illegible]

This image shows a full page of dot grid paper. The dots are arranged in a precise, repeating pattern across the entire surface, providing a guide for writing or drawing without solid lines.

[illegible]

This image shows a full page of white paper with horizontal dotted lines. The lines are evenly spaced and run across the width of the page, providing a guide for handwriting practice. There are no margins, text, or other markings on the page.

[illegible]

[illegible]

This image shows a full page of primary-ruled paper. It features 20 horizontal rows of small, evenly spaced dots, designed to guide young learners in writing their letters and words. The dots are arranged in straight, parallel lines across the entire width of the page.

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[illegible]

This image shows a full page of white paper with horizontal dotted lines. The lines are evenly spaced and run across the width of the page, providing a guide for handwriting practice. There are no margins, text, or other markings on the page.

[illegible]

This image shows a full page of dot grid paper. It features approximately 20 horizontal rows of small, evenly spaced black dots. The dots are arranged in straight lines across the width of the page, providing a guide for writing or drawing without solid lines. The background is white, and there are no margins or other markings present.

[illegible]

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..... **Page 2**

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This image shows a full page of white paper with horizontal dotted lines. The lines are evenly spaced and run across the width of the page, providing a guide for handwriting practice. There are no margins, text, or other markings on the page.

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This image shows a full page of white paper with horizontal dotted lines, typical of primary school writing paper. The lines are evenly spaced and extend across the width of the page. There are no margins, text, or other markings on the paper.

This image shows a full page of dot grid paper. It consists of multiple horizontal rows of small, evenly spaced black dots on a white background. The dots are arranged in straight lines across the width of the page, providing a guide for writing or drawing without solid lines. There are approximately 20 rows of dots visible on the page.

This image shows a full page of dot grid paper. It consists of multiple horizontal rows of small, evenly spaced black dots on a white background. The dots are arranged in straight lines across the entire width of the page, providing a guide for writing or drawing without solid lines.

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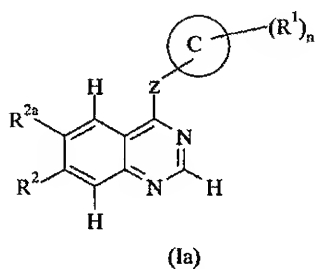
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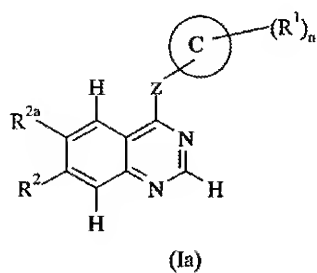
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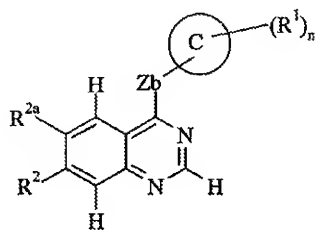
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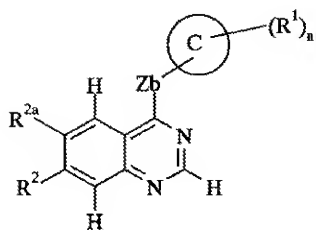
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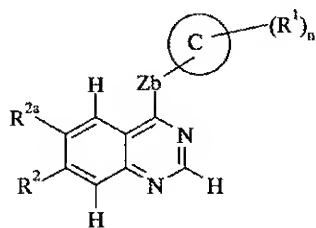
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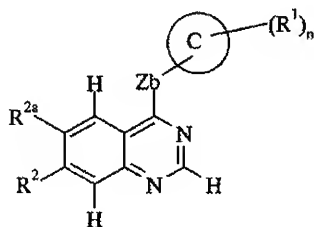
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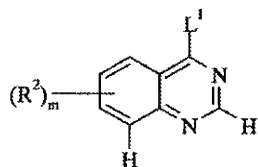
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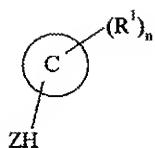
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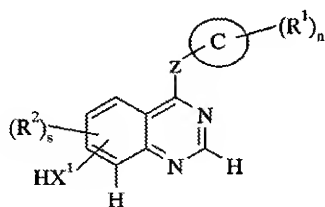
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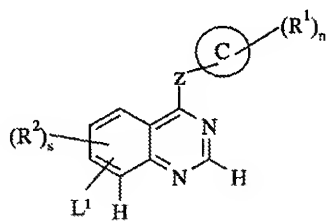
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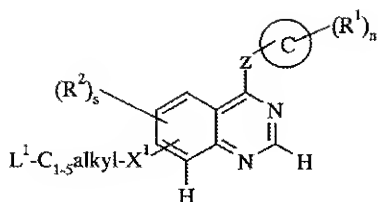


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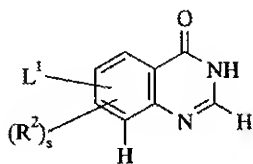
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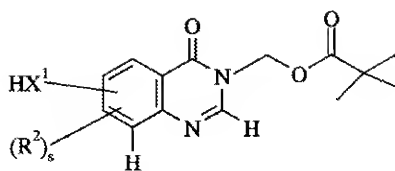
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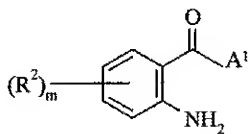
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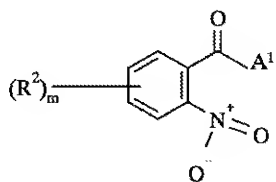
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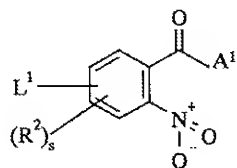
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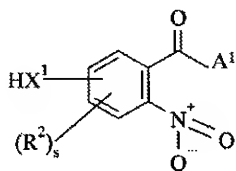
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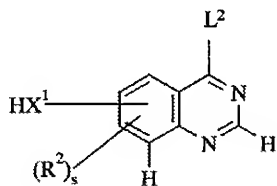
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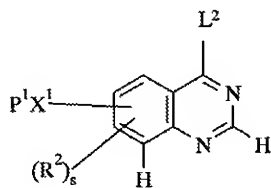
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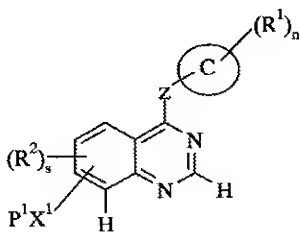
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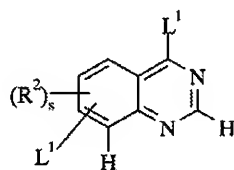
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¹H NMR (CDCl₃): 1.98(m, 2H); 2.40(m, 4H); 2.48(t, 2H); 3.59(m, 4H); 4.00(s, 3H); 4.25(t, 2H); 7.40(s, 1H); 7.58(m, 1H); 7.62(s, 1H); 7.74(dd, 1H); 7.92(d, 1H); 8.10(d, 1H); 8.38(d, 1H); 8.55(s, 1H); 8.92(m, 1H)
MS (ESI): 447 (MH)⁺
元素分析 : 実測値 C 65.9 H 5.7 N 12.4
C₂₅H₂₆N₄O₄ · 0.5H₂O 理論値 C 65.9 H 6.0 N 12.3%

Figure 1 consists of two horizontal dot plots. The top plot is titled 'Number of children per family' and shows a distribution with a peak at 2 children. The bottom plot is also titled 'Number of children per family' and shows a distribution with a peak at 2 children, but with a much larger number of dots at each point, indicating a larger sample size.

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^1H NMR λ° クト λ : (CDCl_3) 4.09(s, 3H); 5.34(s, 2H); 7.42(m, 12H); 7.63(s, 1H)
MS (ESI): 359 (MH) $^+$

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^1H NMR λ° クト λ : (DMSO-d_6) 3.97(s, 3H); 7.22(s, 1H); 7.30(m, 3H); 7.47(t, 2H); 7.56(s, 1H); 8.47(s, 1H); 10.70(s, 1H)
MS (ESI): 269 (MH) $^+$

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^1H NMR λ° クト λ : (DMSO-d_6) 1.85(m, 2H); 2.30(t, 4H); 2.38(t, 2H); 3.53(t, 4H); 3.65(t, 2H)
MS (ESI): 164 (MH) $^+$

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^1H NMR λ^{\wedge} H_2O : (DMSO- d_6) 1.97(m, 2H); 2.39(t, 4H); 2.47(t, 2H); 3.58(t, 4H); 3.95(s, 3H); 4.23(t, 2H); 7.31(m, 3H); 7.36(s, 1H); 7.49(t, 2H); 7.55(s, 1H); 8.52(s, 1H)
MS (ESI): 396 (MH) $^+$

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^1H NMR λ^{\wedge} H_2O : (DMSO- d_6) 1.91(m, 2H); 2.34(t, 4H); 2.42(t, 2H); 3.56(t, 4H); 3.85(s, 3H); 4.12(t, 2H); 7.11(s, 1H); 7.42(s, 1H); 7.96(s, 1H); 12.01(s, 1H)
MS (ESI): 320 (MH) $^+$

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^1H NMR スペクトル: (DMSO-d_6) 1.98(m, 2H); 2.39(m, 4H); 2.48(t, 2H); 3.59(m, 4H); 4.00(s, 3H); 4.25(t, 2H); 7.40(s, 1H); 7.58(m, 2H); 7.62(s, 1H); 7.92(d, 1H); 8.10(d, 1H); 8.44(d, 1H); 8.55(s, 1H); 8.92(m, 1H)

MS (ESI): 447 (MH)⁺

元素分析	:	実測値	C	66.6	H	5.7	N	12.4
$\text{C}_{25}\text{H}_{26}\text{N}_4\text{O}_4 \cdot 0.25\text{H}_2\text{O}$		理論値	C	66.6	H	5.9	N	12.4%

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^1H NMR スペクトル: (DMSO-d_6) 1.98(m, 2H); 2.39(m, 4H); 2.48(t, 2H); 3.59(m, 4H); 4.00(s, 3H); 4.26(t, 2H); 7.40(s, 1H); 7.48(m, 2H); 7.58(m, 2H); 7.74(s, 1H); 7.75(d, 1H); 7.92(d, 1H); 8.03(d, 1H); 8.42(s, 1H)

MS (ESI): 446 (MH)⁺

元素分析	:	実測値	C	69.9	H	6.2	N	9.4
$\text{C}_{26}\text{H}_{27}\text{N}_3\text{O}_4$		理論値	C	70.1	H	6.1	N	9.4%

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MS (ESI): 461 (MH)⁺

$C_{26}H_{28}N_4O_4 \cdot 0.2H_2O$ 理論值 C 67.3 H 6.2 N 12.1%

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^1H NMR スペクトル: (DMSO-d_6) 1.98(m, 2H); 2.65(t, 2H); 2.92(m, 4H); 3.10(m, 4H); 4.00(s, 3H); 4.28(t, 2H); 7.42(s, 1H); 7.58(m, 2H); 7.64(s, 1H); 7.92(d, 1H); 8.10(d, 1H); 8.44(d, 1H); 8.55(s, 1H); 8.92(m, 1H)

MS (ESI): 495 (MH)⁺

元素分析	:	実測値	C	60.0	H	5.0	N	11.1
$\text{C}_{25}\text{H}_{26}\text{N}_4\text{O}_5\text{S} \cdot 0.25\text{H}_2\text{O}$		理論値	C	60.2	H	5.4	N	11.2%

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^1H NMR λ° H_2O : (DMSO- d_6) 3.98(s, 3H); 5.34(s, 2H); 7.42(m, 9H); 7.69(dd, 1H); 8.55(s, 1H)

MS (ESI): 411 (MH) $^+$

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^1H NMR λ° H_2O : (DMSO- d_6) 3.97(s, 3H); 7.22(s, 1H); 7.39(d, 1H); 7.53(m, 2H); 7.67(dd, 1H); 8.46(s, 1H)

MS (ESI): 321 (MH) $^+$

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^1H NMR λ° H_2O : (CDCl $_3$) 1.7-1.8(m, 2H); 2.73(t, 2H); 3.06(br s, 8H); 3.25(s, 1H); 3.78(t, 2H)

MS - ESI: 194 [MH] $^+$

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¹H NMR λ^h ʒ^h ʒ^h (DMSO_d) 1.86(m, 2H); 2.65(t, 2H); 2.92(m, 4H); 3.08(m, 4H); 3.97(s, 3H); 4.26(t, 2H); 7.40(m, 1H); 7.42(s, 1H); 7.56(m, 2H); 7.68(dd, 1H); 8.54(s, 1H)

MS (ESI): 496 (MH)⁺

元素分析	实测值	C	52.7	H	4.4	N	8.3
$C_{22}H_{23}N_3ClFO_5S \cdot 0.25H_2O$	理論值	C	52.8	H	4.7	N	8.4%

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^1H NMR 測定値: (DMSO-d_6) 4.00(s, 3H); 4.00(s, 3H); 7.40(s, 1H); 7.59(m, 3H); 7.92(d, 1H); 8.08(d, 1H); 8.42(d, 1H); 8.55(s, 1H); 8.92(dd, 1H)

MS (ESI): 334 (MH)⁺

元素分析	:	実測値	C	68.2	H	4.3	N	12.5
$\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_3$		理論値	C	68.5	H	4.5	N	12.6%

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^1H NMR スペクトル: (DMSO-d_6) 1.10(m, 1H); 1.51(m, 1H); 1.64(m, 1H); 1.85(m, 3H); 2.09(m, 1H); 2.15(s, 3H); 2.62(m, 1H); 2.82(m, 1H); 3.99(s, 3H); 4.09(d, 2H); 7.38(s, 1H); 7.55(m, 2H); 7.63(s, 1H); 7.91(d, 1H); 8.10(d, 1H); 8.44(d, 1H); 8.54(s, 1H); 8.93(d, 1H)

MS (ESI): 431 (MH)⁺

元素分析	:	実測値	C 68.7	H 5.7	N 12.8
$\text{C}_{25}\text{H}_{26}\text{N}_4\text{O}_3 \cdot 0.3\text{H}_2\text{O}$		理論値	C 68.9	H 6.2	N 12.8%

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^1H NMR $\lambda^\circ\text{ } \delta$ (DMSO- d_6) 1.06(q, 1H); 1.51-1.94(m, 5H); 2.04(s, 3H);
2.34(br s, 1H); 2.62(m, 1H); 2.78(d, 1H); 3.49(m, 1H); 3.59(m, 1H)
MS - ESI: 130 $[\text{MH}]^+$

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^1H NMR $\lambda^\circ\text{ } \delta$ (DMSO- d_6) 1.11(m, 1H); 1.50(m, 1H); 1.58-1.98(m, 4H);
2.09(m, 1H); 2.15(s, 3H); 2.62(d, 1H); 2.81(d, 1H); 3.95(s, 3H); 4.09(d, 2H);
7.39(m, 2H); 7.55(m, 2H); 7.67(d, 1H); 8.53(s, 1H)
MS (ESI): 432 (MH) $^+$

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¹H NMR 3^o 2^o 1^o: (DMSO-d₆) 1.05(m, 1H); 1.40-1.95(m, 5H); 2.02(m, 1H);
2.14(s, 3H); 2.59(d, 1H); 2.78(d, 1H); 3.85(s, 3H); 3.95(d, 2H); 7.09(s, 1H);
7.42(s, 1H); 7.95(s, 1H); 12.00(s, 1H)
MS (ESI): 304 (MH)⁺

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^1H NMR δ (DMSO- d_6): 1.10(m, 1H); 1.42-1.96(m, 5H); 2.09(m, 1H);
2.15(s, 3H); 2.60(d, 1H); 2.80(d, 1H); 3.98(s, 3H); 4.10(d, 2H); 7.35(s, 1H);
7.42(s, 1H); 8.84(s, 1H)
MS (ESI): 322 (MH) $^+$

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^1H NMR スペクトル: (DMSO-d_6 , $\text{CF}_3\text{CO}_2\text{D}$) 1.9-2.0(m, 2H); 2.05-2.2(m, 2H);
2.25-2.4(m, 2H); 2.43(s, 3H); 3.05-3.2(m, 2H); 3.35-3.5(m, 2H); 3.65-3.75(m,
2H); 4.12(s, 3H); 4.35-4.5(t, 2H); 7.0(dd, 1H); 7.35(d, 1H); 7.42(d, 1H); 7.6(s,
1H); 7.85(s, 1H); 9.15(s, 1H)

MS (ESI): 433 (MH)⁺

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^1H NMR スペクトル: (DMSO-d_6 , $\text{CF}_3\text{CO}_2\text{D}$) 2.2(m, 2H); 3.15(t, 2H); 3.3(t, 2H);
3.5(d, 2H); 3.7(t, 2H); 3.82(s, 3H); 4.05(d, 2H); 4.15(t, 2H); 7.07(d, 1H);
7.48(s, 1H); 7.59(d, 1H)

MS - EI: 279 [M]⁺

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^1H NMR スペクトル: (DMSO- d_6 , TFA) 1.8-1.9 (m, 2H); 2.0-2.1 (m, 2H); 2.1-2.2 (m, 2H); 3.0-3.1 (m, 2H); 3.3 (t, 2H); 3.6-3.7 (m, 2H); 3.95 (s, 3H); 4.25 (t, 2H); 7.35 (s, 1H); 7.62 (s, 1H)

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^1H NMR λ° クト℄: (DMSO-d_6 , $\text{CF}_3\text{CO}_2\text{D}$) 1.85-1.95(m, 2H); 2-2.1(m, 2H);
2.15-2.25(m, 2H); 3.0-3.1(m, 2H); 3.31(t, 2H); 3.62(t, 2H); 3.93(s, 3H); 4.2(t,
2H); 7.16(s, 1H); 7.60(s, 1H)
MS - EI: 323 $[\text{M}]^+$

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^1H NMR λ° クト℄: (DMSO-d_6 , $\text{CF}_3\text{CO}_2\text{D}$) 1.9(br s, 2H); 2.05(br s, 2H); 2.2(br s,
2H); 3.05(br s, 2H); 3.3(t, 2H); 3.61(br s, 2H); 3.8(s, 3H); 4.11(t, 2H); 7.05(s,
1H); 7.53(s, 1H)
MS - EI: 293 $[\text{M}]^+$

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¹H NMR (CDCl₃): (DMSO-d₆, CF₃CO₂D) 1.9(m, 2H); 2.0-2.1(m, 2H); 2.2-2.3(m, 2H); 3.05(m, 2H); 3.34(t, 2H); 3.6-3.7(br s, 2H); 3.94(s, 3H); 4.27(t, 2H); 7.31(s, 1H); 7.55(s, 1H); 9.02(s, 1H)

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¹H NMR (λ^o クトル): (CDCl₃) 1.8(br s, 4H); 2.17(m, 2H); 2.6(br s, 4H); 2.7(t, 2H); 4.05(s, 3H); 4.3(t, 2H); 7.35(s, 1H); 7.38(s, 1H); 8.86(s, 1H)
MS - ESI: 322 [MH]⁺

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¹H NMR 8⁺ケトル: (DMSO-d₆) 1.3-1.5(m, 2H); 1.75-1.9(m, 3H); 1.9-2.05(m, 2H); 2.12(s, 3H); 2.8-2.9(d, 2H); 4.5(s, 3H); 4.1(d, 2H); 7.4(s, 1H); 7.6(dd, 1H); 7.62(dd, 1H)
MS (ESI): 431 [MH]⁺

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^1H NMR スペクトル: (CDCl_3) 1.25(t, 3H); 1.45(s, 9H); 1.55-1.70(m, 2H); 1.8-2.0(d, 2H); 2.35-2.5(m, 1H); 2.7-2.95(t, 2H); 3.9-4.1(br s, 2H); 4.15 (q, 2H)

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^1H NMR スペクトル: (CDCl_3) 1.05-1.2(m, 2H); 1.35-1.55(m, 10H); 1.6-1.8(m, 2H); 2.6-2.8(t, 2H); 3.4-3.6(t, 2H); 4.0-4.2(br s, 2H)
MS (EI): 215 $[\text{M}]^+$

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^1H NMR スペクトル: (CDCl_3) 1.0-1.2(m, 2H); 1.45(s, 9H); 1.65(d, 2H); 1.75-1.9(m, 2H); 2.45(s, 3H); 2.55-2.75(m, 2H); 3.85(d, 1H); 4.0-4.2(br s, 2H); 7.35(d, 2H); 7.8(d, 2H)

MS (ESI): 392 $[\text{MNa}]^+$

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^1H NMR スペクトル: (CDCl_3) 1.2-1.35(m, 2H); 1.4(t, 3H); 1.48(s, 9H); 1.8-1.9(d, 2H); 2.0-2.15(m, 2H); 2.75(t, 2H); 3.9(d, 2H); 3.95(s, 3H); 4.05-4.25(br s, 2H); 4.35(q, 2H); 6.85(d, 1H); 7.55(s, 1H); 7.65(d, 1H)

MS (ESI): 416 $[\text{MNa}]^+$

元素分析	:	実測値	C	63.4	H	8.0	N	3.5
$\text{C}_{21}\text{H}_{31}\text{NO}_6 \cdot 0.3\text{H}_2\text{O}$		理論値	C	63.2	H	8.0	N	3.5%

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^1H NMR λ° fff : (DMSO-d_6) 1.3(t, 3H); 1.45-1.65(m, 2H); 1.75-2.1(m, 3H);
 2.75(s, 3H); 2.9-3.05(m, 2H); 3.4-3.5(d, 2H); 3.95(s, 3H); 4.05(d, 2H); 4.3(q,
 2H); 7.32(s, 1H); 7.66(s, 1H)
 MS (ESI): 353 $[\text{MH}]^+$

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m.p. 111-112°C

^1H NMR λ° fff : (CDCl_3) 1.35(t, 3H); 1.4-1.5(m, 2H); 1.85(m, 3H); 1.95(t,
 2H); 2.29(s, 3H); 2.9(d, 2H); 3.8(s, 3H); 3.85(d, 2H); 4.3(q, 2H); 5.55(br s,
 2H); 6.13(s, 1H); 7.33(s, 1H)

MS (ESI): 323 $[\text{MH}]^+$

元素分析	:	実測値	C	62.8	H	8.5	N	8.3
$\text{C}_{17}\text{H}_{26}\text{N}_2\text{O}_4 \cdot 0.2\text{H}_2\text{O}$		理論値	C	62.6	H	8.2	N	8.6%

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^1H NMR λ° DMSO-d_6) 1.25-1.4(m, 2H); 1.75(d, 2H); 1.9(t, 1H); 1.9(s, 3H); 2.16(s, 2H); 2.8(d, 2H); 3.9(s, 3H); 4.0(d, 2H); 7.11(s, 1H); 7.44(s, 1H); 7.97(s, 1H)

MS (ESI): 304 $[\text{MH}]^+$

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^1H NMR δ (DMSO- d_6): 1.3-1.5(m, 2H); 1.75-1.9(m, 3H); 2.0(t, 1H);
 2.25(s, 3H); 2.85(d, 2H); 4.02(s, 3H); 4.12(d, 2H); 7.41(s, 1H); 7.46(s, 1H);
 8.9(s, 1H)
 MS (ESI): 322 [MH] $^+$

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^1H NMR δ (DMSO- d_6): 1.3-1.45(m, 2H); 1.7-1.95(m, 5H); 2.15(s, 3H);
 2.4(s, 3H); 2.8(d, 2H); 3.98(s, 3H); 4.05(d, 2H); 6.14(s, 1H); 6.88(d, 1H);
 7.29(s, 1H); 7.32(d, 1H); 7.35(s, 1H); 7.6(s, 1H); 8.45(s, 1H)
 MS (ESI): 433 [MH] $^+$

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^1H NMR スペクトル: (DMSO-d_6) 1.3-1.45(m, 2H); 1.75-1.9(m, 3H); 2.05(t, 2H); 2.72(t, 2H); 2.95(d, 2H); 3.05(s, 3H); 3.35-3.45(m, 2H); 4.00(s, 3H); 4.1(d, 2H); 7.41(s, 1H); 7.57(dd, 1H); 7.62(dd, 1H); 7.65(s, 1H); 7.93(s, 1H); 8.12(d, 1H); 8.45(d, 1H); 8.55(s, 1H); 8.95(d, 1H)

MS (ESI): 523 [MH] $^+$

元素分析	:	実測値	C	61.3	H	6.0	N	10.6
$\text{C}_{27}\text{H}_{30}\text{N}_4\text{O}_5\text{S} \cdot 0.4\text{H}_2\text{O}$		理論値	C	61.2	H	5.9	N	10.6%

^1H NMR λ° DMSO-d_6) 1.11(s, 9H); 3.89(s, 3H); 5.3(s, 2H); 5.9(s, 2H);
7.27(s, 1H); 7.35(m, 1H); 7.47(t, 2H); 7.49(d, 2H); 7.51(s, 1H); 8.34(s, 1H)

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^1H NMR λ° DMSO-d_6) 1.1(s, 9H); 3.89(s, 3H); 5.89(s, 2H); 7.0(s, 1H);
7.48(s, 1H); 8.5(s, 1H)

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^1H NMR λ° g t : (DMSO- d_6) 1.1(s, 9H); 1.1-1.3(m, 2H); 1.42(s, 9H); 1.73(d, 2H); 1.93-2.1(br s, 1H); 2.65-2.9(br s, 2H); 3.9(s, 3H); 3.9-4.1(m, 4H); 5.9(s, 2H); 7.2(s, 1H); 7.5(s, 1H); 8.35(s, 1H)

MS (ESI): 526 [MNa] $^+$

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^1H NMR λ° g t : (DMSO- d_6 , $\text{CF}_3\text{CO}_2\text{D}$) 1.15(s, 9H); 1.5-1.7(m, 2H); 2.0(d, 2H); 2.2-2.3(br s, 1H); 3.0(t, 2H); 3.4(d, 2H); 3.94(s, 3H); 4.15(d, 2H); 5.97(s, 2H); 7.3(s, 1H); 7.6(s, 1H); 8.65(s, 1H)

MS (ESI): 404 [MH] $^+$

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^1H NMR λ° ftf : (DMSO-d_6) 1.09(s, 9H); 1.25-1.4(m, 2H); 1.7-1.9(m, 3H);
2.0(t, 2H); 2.7(t, 2H); 2.95(d, 2H); 3.02(s, 3H); 3.25-3.45(m, 2H); 3.9(s, 3H);
4.0(d, 2H); 5.9(s, 2H); 7.15(s, 1H); 7.49(s, 1H); 8.35(s, 1H)
MS (ESI): 510 $[\text{MH}]^+$.

^1H NMR λ° ftf : (DMSO-d_6) 1.2-1.4(m, 2H); 1.7-1.85(m, 3H); 2.0(t, 2H);
2.7(t, 2H); 2.9(d, 2H); 3.02(s, 3H); 3.3-3.5(m, 2H); 3.9(s, 3H); 4.0(d, 2H);
7.11(s, 1H); 7.45(s, 1H); 7.97(s, 1H)
MS (ESI): 396 $[\text{MH}]^+$

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MS (ESI): 414 [MH]⁺

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MS (ESI): 445 [MH]⁺

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MS (ESI): 525 [MH]⁺

元素分析	:	実測値	C 60.7	H 6.2	N 10.5
$C_{27}H_{32}O_5S \cdot 0.5H_2O$:	理論値	C 60.8	H 6.2	N 10.5%

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^1H NMR λ^{\wedge} クトル: (DMSO- d_6) 1.7(br s, 4H); 2.05(m, 2H); 2.5(br s, 4H); 2.6(t, 2H); 2.75(s, 3H); 4.02(s, 3H); 4.3(t, 2H); 7.41(s, 1H); 7.45(d, 1H); 7.65(s, 1H); 7.65(d, 1H); 7.95(s, 1H); 8.25(d, 1H); 8.55(s, 1H); 8.8(d, 1H)

MS (ESI): 445 [MH] $^+$

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^1H NMR λ^{\wedge} クトル: (DMSO- d_6) 1.23(s, 6H); 1.7(br s, 4H); 1.85(s, 3H); 2.0(m, 2H); 2.45(br s, 4H); 2.57(t, 2H); 3.95(s, 3H); 4.25(t, 2H); 5.35(s, 1H); 5.9(s, 1H); 6.5(d, 1H); 6.8(dd, 1H); 6.85(s, 1H); 7.32(s, 1H); 7.52(s, 1H); 8.5(s, 1H)

MS (ESI): 475 [MH] $^+$

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¹H NMR (δ, CDCl₃): 1.25-1.45(m, 2H); 1.8(d, 2H); 1.7-1.9(m, 1H); 1.9(t, 2H); 2.2(s, 3H); 2.8(d, 2H); 3.97(s, 3H); 4.05(d, 2H); 4.65(s, 2H); 6.8(s, 1H); 6.85(d, 1H); 7.05(d, 1H); 7.35(s, 1H); 7.52(s, 1H); 8.55(s, 1H)
MS (ESI): 451 [MH]⁺

¹H NMR (λ⁶ 400 MHz): (DMSO-d₆, CF₃CO₂D) 1.8-2.0(m, 2H); 2.0-2.15(m, 2H); 2.2-2.35(m, 2H); 3.0-3.2(m, 2H); 3.4(t, 2H); 3.6-3.75(m, 2H); 4.05(s, 3H); 4.35(t, 2H); 4.65(s, 2H); 6.85(s, 1H); 6.9(d, 1H); 7.1(d, 1H); 7.5(s, 1H); 7.7(s, 1H); 8.9(s, 1H)
MS (ESI): 451 [MH]⁺

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¹H NMR スペクトル: (DMSO-d₆) 1.3-1.5(m, 2H); 1.8(d, 2H); 1.9(t, 2H); 1.8-1.9(m, 1H); 2.2(s, 3H); 2.82(d, 2H); 4.02(s, 3H); 4.1(d, 2H); 7.4(s, 1H); 7.6(dd, 1H); 7.65(s, 1H); 7.75(d, 1H); 7.95(s, 1H); 8.15(d, 1H); 8.4(d, 1H); 8.55(s, 1H); 8.95(d, 1H)

MS (ESI): 431 [MH]⁺

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[illegible]

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^1H NMR λ^\wedge κ τ β : (DMSO-d_6 , $\text{CF}_3\text{CO}_2\text{D}$) 2.3(m, 2H); 3.2(m, 2H); 3.4(m, 2H); 3.5(m, 2H); 3.7(m, 2H); 4.0(m, 2H); 4.1(s, 3H); 4.4(m, 2H); 7.55(s, 1H); 7.75(s, 1H); 7.90(dd, 1H); 7.95(d, 1H); 8.15(d, 1H); 8.45 (d, 1H); 8.80(s, 1H); 9.05(d, 1H)

MS - ESI: 481 [MH] $^+$

元素分析	:	実測値	C	61.8	H	5.1	N	11.5
$\text{C}_{25}\text{H}_{25}\text{ClN}_4\text{O}_4$		理論値	C	62.4	H	5.2	N	11.7%

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^1H NMR λ^\wedge κ τ β : (DMSO-d_6) 7.37(s, 1H); 7.39(d, 1H); 7.62(d, 1H); 8.15(d, 1H); 8.8(d, 1H)

MS - EI: m/z 179 [M.] $^+$

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¹H NMR (400 MHz, DMSO-d₆): 2.3-2.4 (m, 2H), 3.05-3.2 (m, 2H), 3.25-3.35 (m, 2H), 3.5 (d, 2H), 3.82 (t, 2H), 4.0 (d, 2H), 4.05 (s, 3H), 4.32 (t, 2H), 6.1 (s, 2H), 7.02 (d, 1H), 7.1 (dd, 1H), 7.3 (s, 1H), 7.4 (s, 1H), 8.32 (s, 1H), 8.8 (s, 1H)

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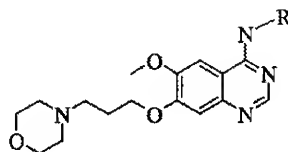
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表 I

実施例 番号	重量 (mg)	収量%	MS-ESI [MH] ⁺	註	R
25	104	90	435.1	a	1- <i>H</i> -イミダゾール-6-イル
26	102	89	435.1	b	1- <i>H</i> -イミダゾール-5-イル
27	99	84	452	c	1,3-ベンゾチアゾール-6-イル
28	108	91	466	d	2-メチル-1,3-ベンゾチアゾール-5-イル
29	102	95	435.1	e	2,3-ジヒドロ-1 <i>H</i> -インデン-5-イル

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^1H NMR λ° C_6D_6 : (DMSO- d_6) 2.3-2.4 (m, 2H), 3.05-3.2 (m, 2H), 3.2-3.3 (m, 2H), 3.52 (d, 2H), 3.85 (t, 2H), 4.0 (d, 2H), 4.05 (s, 3H), 4.32 (t, 2H), 7.42 (s, 1H), 7.45 (d, 1H), 7.85 (d, 1H), 7.98 (s, 1H), 8.1 (s, 1H), 8.42 (s, 1H), 8.85 (s, 1H)

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^1H NMR λ° C_6D_6 : (DMSO- d_6) 2.3-2.4 (m, 2H), 3.05-3.2 (m, 2H), 3.25-3.3 (m, 2H), 3.45-3.55 (m, 2H), 3.8-3.9 (m, 2H), 3.9-4.02 (m, 2H), 4.05 (s, 3H), 4.32 (t, 2H), 7.42 (s, 1H), 7.65 (m, 2H), 8.05 (s, 1H), 8.15 (s, 1H), 8.4 (s, 1H), 8.75 (s, 1H)

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^1H NMR λ° C_6D_6 : (DMSO- d_6) 2.3-2.4 (m, 2H), 3.05-3.2 (m, 2H), 3.2-3.3 (m, 2H), 3.55 (d, 2H), 3.8 (t, 2H), 4.0 (d, 2H), 4.08 (s, 3H), 4.32 (t, 2H), 7.4 (s, 1H), 7.88 (dd, 1H), 8.2 (d, 1H), 8.4 (s, 1H), 8.55 (s, 1H), 8.85 (s, 1H), 9.42 (s, 1H)

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^1H NMR λ° C_6H_6 : (DMSO- d_6) 2.3-2.4 (m, 2H), 2.85 (s, 3H), 3.05-3.2 (m, 2H),
3.3 (t, 2H), 3.4-3.5 (m, 2H), 3.85 (t, 2H), 4.0 (d, 2H), 4.05 (s, 3H), 4.35 (t, 2H),
7.42 (s, 1H), 7.75 (dd, 1H), 8.15 (d, 1H), 8.3 (s, 1H), 8.42 (s, 1H), 8.85 (s, 1H)

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^1H NMR λ° C_6H_6 : (DMSO- d_6) 2.08 (m, 2H), 2.3-2.4 (m, 2H), 2.9 (m, 4H), 3.05-
3.2 (m, 2H), 3.2-3.3 (m, 2H), 3.5 (d, 2H), 3.82 (t, 2H), 4.0 (d, 2H), 4.05 (s, 3H),
4.3 (t, 2H), 7.32 (d, 1H), 7.4 (m, 2H), 7.55 (s, 1H), 8.32 (s, 1H), 8.8 (s, 1H)

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MS - ESI: 462 [MH]⁺

¹H NMR スペクトル: (DMSO-d₆) 1.3-1.5 (m, 2H); 1.75-1.95 (m, 5H); 2.2 (s, 3H), 2.42 (s, 3H); 4.0 (s, 3H); 4.1 (d, 2H); 6.3 (s, 2H); 7.4 (s, 1H); 7.45 (dd, 1H); 7.6 (s, 1H); 7.7 (s, 1H); 8.15 (d, 1H); 8.61 (s, 1H)

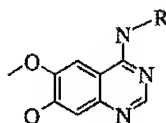


表 II

実施例 番号	重量 (mg)	収量 %	MS-ESI [MH] ⁺	註	Q	R
31	180	85	451	a	1-メチルピペリジン- 4-イルメトキシ	4-メチル-3,4-ジヒドロ-2H- 1,4-ベンゾキサジン-6-イルオキシ
32	160	87	462	b	3-ピロリジン-1- イルプロポキシ	2-メチル-4-オキシ-4H- クロメン-7-イルオキシ
33	100	56	451	c	3-ピロリジン-1- イルプロポキシ	4-メチル-3,4-ジヒドロ-2H- 1,4-ベンゾキサジン-6-イルオキシ

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^1H NMR λ° H_2O : (DMSO- d_6) 1.6-1.75 (m, 2H); 1.9-2.3 (m, 5H); 2.8 (s, 3H);
2.9 (s, 3H); 3.0-3.15 (m, 2H); 3.3 (br s, 2H); 3.5-3.6 (d, 2H); 4.1 (s, 3H); 4.2 (d,
2H); 4.3 (t, 2H); 6.55 (m, 1H); 6.75 (s, 1H); 6.8 (d, 1H); 7.6 (s, 1H); 7.75 (s,
1H); 9.15 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6 , CF_3COOD) 1.8-2.0 (m, 2H); 2.0-2.15 (m, 2H);
2.2-2.3 (m, 2H); 2.4 (s, 3H); 3.05-3.15 (m, 2H); 3.3-3.4 (m, 2H); 3.6-3.7 (m,
2H); 4.05 (s, 3H); 4.35 (t, 2H); 6.3 (s, 1H); 7.45 (d, 1H); 7.5 (s, 1H); 7.65 (s,
1H); 7.72 (s, 1H); 8.15 (d, 1H); 8.75 (s, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 1.85-2.0 (m, 2H); 2.0-2.15 (m, 2H); 2.25-2.35 (m, 2H); 2.83 (s, 3H); 3.05-3.15 (m, 2H); 3.3 (t, 2H); 3.4 (t, 2H); 3.7 (br m, 2H); 4.1 (s, 3H); 4.3 (t, 2H); 4.4 (t, 2H); 6.52 (d, 1H); 6.7 (s, 1H); 6.8 (d, 1H); 7.55 (s, 1H); 7.75 (s, 1H); 9.1 (s, 1H)

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MS - ESI: 419 $[\text{MH}]^+$

^1H NMR λ° H_2O : (DMSO-d_6) 1.35-1.5 (m, 2H); 1.8 (d, 2H); 1.95 (t, 2H); 1.7-2.0 (m, 1H); 2.2 (s, 3H); 2.85 (d, 2H); 4.02 (s, 3H); 4.1 (d, 2H); 6.45 (s, 1H); 7.0 (d, 1H); 7.35 (s, 1H); 7.4-7.5 (m, 3H); 7.6 (s, 1H); 8.5 (s, 1H)

元素分析	:	実測値	C	67.4	H	6.5	N	13.1
$\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_3 \cdot 0.5\text{H}_2\text{O}$		理論値	C	67.4	H	6.4	N	13.1%

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MS - ESI: 447 [MH]⁺

¹H NMR スペクトル: (DMSO-d₆) 1.2-1.4 (m, 2H); 1.7 (d, 2H); 1.8 (t, 2H); 1.7-1.9 (m, 1H); 2.05 (s, 3H); 2.12 (s, 3H); 2.25 (s, 3H); 2.75 (d, 2H); 3.9 (s, 3H); 4.0 (d, 2H); 6.8 (d, 1H); 7.15 (s, 1H); 7.2 (d, 1H); 7.3 (s, 1H); 7.52 (s, 1H); 8.45 (s, 1H)

元素分析	:	実測値	C	68.6	H	6.9	N	12.5
C ₂₆ H ₃₀ N ₄ O ₃ · 0.4H ₂ O		理論値	C	68.8	H	6.8	N	12.4%

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MS - ESI 419 [MH]⁺

¹H NMR 測定値: (DMSO-d₆, CF₃COOD) 1.9-2.0 (m, 2H); 2.1 (m, 2H); 2.3 (t, 2H); 3.0-3.15 (m, 2H); 3.4 (t, 2H); 3.6-3.75 (m, 2H); 4.1 (s, 3H); 4.4 (t, 2H); 6.5 (s, 1H); 7.05 (d, 1H); 7.5 (s, 1H); 7.5-7.6 (m, 2H); 7.85 (s, 1H); 9.11 (s, 1H)

元素分析	:	実測値	C	63.7	H	6.4	N	12.1
C ₂₄ H ₂₆ N ₄ O ₃ · 1.9H ₂ O		理論値	C	63.7	H	6.6	N	12.4%

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MS - ESI: 446 [MH]⁺

¹H NMR 測定値: (DMSO-d₆): 1.8-1.9 (m, 2H); 2.0 (d, 2H); 2.1-2.2 (m, 1H); 2.16 (s, 3H); 2.33 (s, 3H); 2.75 (br s, 3H); 2.95-3.05 (m, 2H); 3.5 (d, 2H); 4.0 (s, 3H); 4.07 (d, 2H); 7.25 (d, 1H); 7.4 (d, 1H); 7.42 (s, 1H); 7.52 (s, 1H); 8.25 (s, 1H); 8.75 (s, 1H); 10.0 (br s, 1H); 10.9 (s, 1H); 11.25 (br s, 1H)

元素分析	:	実測値	C	58.5	H	6.8	N	12.9
C ₂₆ H ₃₁ N ₅ O ₂ · 1H ₂ O · 1.9HCl		理論値	C	58.6	H	6.6	N	13.1%

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MS - ESI: 446 [MH]⁺

¹H NMR 測定値: (DMSO-d₆, CF₃COOD) 1.85-2.0 (m, 2H); 2.05-2.15 (m, 2H);
2.1 (s, 3H); 2.2 (s, 3H); 2.25-2.35 (m, 2H); 2.35 (s, 3H); 3.0-3.15 (m, 2H);
3.32-3.42 (m, 2H); 3.6-3.7 (m, 2H); 4.05 (s, 3H); 4.3 (t, 2H); 7.2 (d, 1H); 7.3 (s,
1H); 7.35 (d, 1H); 7.57 (s, 1H); 8.2 (s, 1H); 8.8 (s, 1H)

元素分析 : 実測値 C 58.8 H 7.0 N 12.5

C₂₆H₃₁N₅O 1.9H₂O 1.9HCl 0.1 水分子 理論値 C 58.6 H 7.1 N 12.9%

MS - ESI: 432 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.8-1.9 (m, 2H); 2.0-2.1 (m, 2H); 2.15-2.35 (m,
2H); 2.4 (s, 3H); 3.0-3.1 (m, 2H); 3.2-3.3 (m, 2H); 3.5-3.6 (m, 2H); 4.0 (s, 3H);
4.32 (t, 2H); 6.2 (s, 1H); 7.2 (d, 1H); 7.3 (m, 2H); 7.65 (s, 1H); 8.25 (s, 1H);
8.75 (s, 1H); 10.75 (br s, 1H); 11.15 (s, 1H); 11.25 (br s, 1H)

元素分析 : 実測値 C 58.9 H 6.6 N 13.5

C₂₅H₂₉N₅O₂ 2.2HCl 0.1 水分子 理論値 C 58.7 H 6.2 N 13.5%

MS - ESI: 432 [MH]⁺

¹H NMR 測定値: (DMSO-d₆, CF₃COOD) 1.5-1.7 (m, 2H); 2.05 (d, 2H); 2.1-2.2 (m, 1H); 2.45 (s, 3H); 2.8 (s, 3H); 3.05 (t, 2H); 3.5 (d, 2H); 4.0 (s, 3H); 4.1 (d, 2H); 6.2 (s, 1H); 7.2 (d, 1H); 7.32 (d, 1H); 7.4 (d, 1H); 7.6 (s, 1H); 8.2 (s, 1H); 8.85 (s, 1H)

元素分析	:	実測値	C 53.9	H 6.8	N 12.4
C ₂₅ H ₂₉ N ₅ O ₂ · 2.6H ₂ O · 2.07HCl		理論値	C 54.2	H 6.6	N 12.6%

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MS - ESI: 445 [MH]⁺

¹H NMR 測定値: (CDCl₃) 1.8 (br s, 4H); 2.2 (m, 2H); 2.5 (br s, 4H); 2.7 (t, 2H); 2.8 (s, 3H); 4.1 (s, 3H); 4.3 (t, 2H); 7.3 (d, 1H); 7.35 (s, 1H); 7.45 (dd, 1H); 7.6 (s, 1H); 7.85 (d, 1H); 7.9 (s, 1H); 8.1 (d, 1H); 8.6 (s, 1H)

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MS - ESI: 537 [MH]⁺

¹H NMR スペクトル: (DMSO-d₆) 1.3-1.5 (m, 2H); 1.75-1.95 (m, 3H); 1.95-2.15 (m, 2H); 2.7 (s, 3H); 2.7-2.8 (m, 2H); 2.9-3.0 (m, 2H); 3.05 (s, 3H); 3.2-3.35 (m, 2H); 4.02 (s, 3H); 4.1 (d, 2H); 7.4 (s, 1H); 7.45 (d, 1H); 7.55 (d, 1H); 7.65 (s, 1H); 7.8 (s, 1H); 8.05 (d, 1H); 8.35 (d, 1H); 8.55 (s, 1H)

元素分析 : 実測値 C 62.2 H 6.3 N 10.4

C₂₈H₃₂N₄O₅S 0.35 エーテル 0.2DMF 理論値 C 62.4 H 6.4 N 10.2%

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MS - ESI: 487 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.25-1.4 (m, 2H); 1.75 (d, 2H); 1.8 (t, 2H); 1.7-2.0 (m, 1H); 2.2 (s, 3H); 2.75 (d, 2H); 4.0 (s, 3H); 4.1 (d, 2H); 7.0 (s, 1H); 7.25 (d, 1H); 7.4 (s, 1H); 7.6 (d, 1H); 7.8 (s, 1H); 8.5 (s, 1H); 12.5 (s, 1H)

元素分析	:	実測値	C 60.2	H 5.8	N 10.9
C ₂₅ H ₂₅ F ₃ N ₄ O ₃ · 0.7H ₂ O · 0.2 I-イオン		理論値	C 60.3	H 5.6	N 10.9%

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¹H NMR 測定値: (CDCl₃) 3.83 (s, 3H), 6.82 (s, 1H), 7.0 (dd, 1H), 7.1 (s, 1H), 7.3 (d, 1H), 8.15 (br s, 1H)

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¹H NMR (δ, CDCl₃): 4.64 (s, 1H), 6.8 (s, 1H), 6.92 (dd, 1H), 7.1 (s, 1H), 7.3 (d, 1H), 8.3 (br s, 1H)

元素分析	：	実測値	C 53.3	H 2.9	N 6.8
$C_9H_6F_3NO \cdot 0.1 H_2O$		理論値	C 53.3	H 3.1	N 6.9%

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MS - ESI: 487 [MH]⁺

¹H NMR スペクトル: (CDCl₃) 1.8 (m, 4H); 2.1-2.3 (m, 2H); 2.55 (br s, 4H); 2.7 (t, 2H); 4.1 (s, 3H); 4.3 (t, 2H); 6.95 (s, 1H); 7.2 (dd, 1H); 7.35 (s, 1H); 7.5 (d, 1H); 7.55 (s, 1H); 7.6 (s, 1H); 8.6 (s, 1H); 8.8 (s, 1H)

元素分析	:	実測値	C	61.7	H	5.5	N	11.5
C ₂₅ H ₂₅ F ₃ N ₄ O ₃		理論値	C	61.7	H	5.2	N	11.5%

MS - ESI: 445 [MH]⁺

¹H NMR スペクトル: (CDCl₃) 1.4-1.6 (m, 2H); 1.95 (d, 2H); 2.05 (t, 2H); 1.9-2.1 (m, 1H); 2.35 (s, 3H); 2.8 (s, 3H); 2.95 (d, 2H); 4.1 (s, 3H); 4.15 (d, 2H); 7.3 (m, 2H); 7.45 (dd, 1H); 7.6 (s, 1H); 7.9 (d, 1H); 7.95 (s, 1H); 8.1 (d, 1H); 8.6 (s, 1H)

元素分析	:	実測値	C	69.7	H	6.5	N	12.8
C ₂₆ H ₂₆ N ₄ O ₃ · 0.2H ₂ O		理論値	C	69.7	H	6.4	N	12.5%

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MS - ESI: 447 [MH]⁺

¹H NMR 測定値: (DMSO-d₆, CF₃COOD) 1.9-2.0 (m, 2H); 2.05-2.15 (m, 2H);
 2.15 (s, 3H); 2.3-2.4 (m, 2H); 2.4 (s, 3H), 3.05-3.15 (m, 2H); 3.35-3.45 (t, 2H);
 3.7 (br s, 2H); 4.1 (s, 3H); 4.4 (t, 2H); 6.95 (d, 1H); 7.3 (s, 1H); 7.35 (d, 1H);
 7.55 (s, 1H); 7.85 (s, 1H); 9.15 (s, 1H)

元素分析	:	実測値	C	67.7	H	6.8	N	12.2
C ₂₆ H ₃₀ N ₄ O ₃ · 0.8H ₂ O		理論値	C	67.8	H	6.9	N	12.2%

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MS - ESI: 412 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 2.4 (s, 3H); 4.0 (s, 3H); 5.35 (s, 2H); 6.15 (s,
 1H); 6.85 (s, 1H); 7.2-7.6 (m, 9H); 8.5 (s, 1H)

元素分析	:	実測値	C	72.2	H	5.1	N	10.2
C ₂₅ H ₂₁ N ₃ O ₃ · 0.2H ₂ O		理論値	C	72.3	H	5.2	N	10.1%

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^1H NMR λ° ʒ ʒ ʒ: (DMSO d_6) 2.35 (s, 3H) ; 5.95 (s, 1H) ; 6.5 (dd, 1H) ; 6.7 (s, 1H) ; 7.05 (d, 1H) ; 8.5 (s, 1H)

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MS - ESI: 322 [MH] $^{+}$

^1H NMR λ° ʒ ʒ ʒ: (DMSO d_6) 2.4 (s, 3H); 4.0 (s, 3H); 6.15 (s, 1H); 6.9 (d, 1H); 7.2 (s, 1H); 7.25 (s, 1H); 7.3 (d, 1H); 7.6 (s, 1H); 8.4 (s, 1H)

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MS - ESI: 496 [MH]⁺

¹H NMR λ[°] ʁʁʁ: (DMSO-d₆, CF₃COOD) 2.25-2.4 (m, 2H), 3.1 (s, 3H), 3.35 (t, 2H), 4.1 (s, 3H), 4.4 (t, 2H), 7.1 (s, 1H), 7.3 (d, 1H), 7.5 (s, 1H), 7.6 (d, 1H), 7.7 (s, 1H), 7.78 (s, 1H), 8.9 (s, 1H)

¹H NMR λ[°] ʁʁʁ: (CDCl₃) 2.10(m, 2H); 2.96(s, 3H); 3.20(t, 2H); 3.80(t, 2H)

MS - ESI: 139 [MH]⁺

¹H NMR 300 MHz (CDCl₃): 1.2(s, 9H); 2.4-2.5(m, 2H); 3.0(s, 3H); 3.25-3.35(t, 2H); 5.95(s, 1H); 7.1(s, 1H); 7.65(s, 1H); 8.2(s, 1H)

[illegible]

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^1H NMR λ^{\wedge} H : (DMSO-d_6) 2.2-2.3(m, 2H); 3.05(s, 3H); 3.35(t, 2H); 3.9(s, 3H); 4.25(t, 2H); 7.15(s, 1H); 7.5(s, 1H); 8.0(s, 1H)

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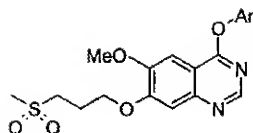
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表 Ⅲ



実施例 番号	重量 (mg)	収量 %	MS-ESI [MH] ⁺	Ar	註
51	189	92	454	2-メチルキリリン-7-イル	a
52	175	90	428	インドール-5-イル	b

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¹H NMR スペクトル: (DMSO-d₆, CF₃COOD) 2.2-2.35 (m, 2H), 2.95 (s, 3H), 3.1 (s, 3H), 3.35 (m, 2H), 4.05 (s, 3H), 4.4 (t, 2H), 7.5 (s, 1H), 7.7 (s, 1H), 7.95 (dd, 1H), 8.02 (d, 1H), 8.2 (s, 1H), 8.48 (d, 1H), 8.7 (s, 1H), 9.12 (d, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 2.2-2.35 (m, 2H), 3.1 (s, 3H), 3.3-3.4 (t, 2H), 4.0 (s, 3H), 4.4 (t, 2H), 6.5 (s, 1H), 7.0 (dd, 1H), 7.4 (s, 1H), 7.4-7.5 (m, 3H), 7.6 (s, 1H), 8.5 (s, 1H), 11.25 (s, 1H)

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MS - ESI: 393 $[\text{MH}]^+$

^1H NMR λ° H_2O : (DMSO-d_6) 2.25 (s, 6H), 2.4 (s, 3H), 2.75 (t, 2H), 4.0 (s, 3H), 4.3 (t, 2H), 6.15 (s, 1H), 6.87 (d, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 7.5 (s, 1H)

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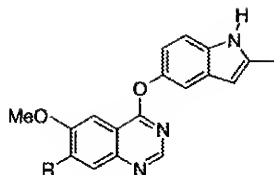
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表 IV



実施例 番号	重量 (mg)	収量 %	MS-ESI [MH] ⁺	R	註
54	25	17	419	2-ピロリジン-1-イルエトキシ	a
55	112	74	433	1-メチルピペリジン-3-イルメトキシ	b
56	115	72	456	2-(N-メチル-N-(4-ピリジル)アミノ)エトキシ	c

¹H NMR スペクトル: (DMSO-d₆) 1.65-1.8 (m, 4H), 2.4 (s, 3H), 2.6 (br s, 4H), 2.9 (t, 2H), 4.0 (s, 3H), 4.3 (t, 2H), 6.15 (s, 1H), 6.9 (d, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

^1H NMR λ° H_2O : (DMSO-d_6) 1.45-2.2 (m, 7H), 2.18 (s, 3H), 2.4 (s, 3H), 2.6 (br d, 1H), 2.85 (br d, 1H), 4.0 (s, 3H), 4.1 (d, 2H), 6.15 (s, 1H), 6.9 (d, 1H), 7.25 (d, 1H), 7.3 (d, 1H), 7.35 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 2.4 (s, 3H), 3.1 (s, 3H), 3.9 (t, 2H), 3.97 (s, 3H), 4.4 (t, 2H), 6.15 (s, 1H), 6.75 (d, 2H), 6.87 (dd, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.35 (s, 1H), 7.6 (s, 1H), 8.15 (d, 2H), 8.5 (s, 1H)

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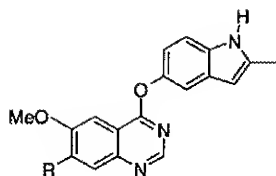
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表 V



実施例 番号	重量 (mg)	収量 %	MS-ESI [MH] ⁺	R	註
57	115	76	435	2-モルホリノエトキシ	a
58	64	42	433	2-ピペリジノエトキシ	b
59	66	43	437	2-(N-(2-メトキシエチル)-N- メチルアミノ)エトキシ	c
60	118	75	449	3-モルホリノプロポキシ	d
61	101	68	424	2-(2-メトキシエトキシ)エトキシ	e
62	81	57	407	3-(N,N-ジメチルアミノ)プロポキシ	f
63	160	92	497	3-(1,1-ジオキソチオモルホリノ)プロポキシ	g
64	121	83	417	2-(1H-1,2,4-トリアゾール-1-イル)エトキシ	h
65	38	22	492	2-(2-(4-メチルピペラジン-1- イル)エトキシ)エトキシ	i
66	80	48	479	2-(2-モルホリノエトキシ)エトキシ	j

¹H NMR スペクトル: (DMSO-d₆) 2.4 (s, 3H), 2.5-2.7 (m, 4H), 2.8 (t, 2H), 3.6 (t, 4H), 4.0 (s, 3H), 4.35 (t, 2H), 6.15 (s, 1H), 6.87 (dd, 1H), 7.25 (s, 1H), 7.32 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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^1H NMR スペクトル: (DMSO-d_6) 1.3-1.45 (m, 2H), 1.4-1.6 (m, 4H), 2.4 (s, 3H),
2.4-2.5 (m, 4H), 2.75 (t, 2H), 3.97 (s, 3H), 4.3 (t, 2H), 6.15 (s, 1H), 6.9 (d, 1H),
7.25 (s, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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^1H NMR スペクトル: (DMSO-d_6) 2.35 (s, 3H), 2.4 (s, 3H), 2.65 (t, 2H), 2.85 (t,
2H), 3.25 (s, 3H), 3.45 (t, 2H), 3.97 (s, 3H), 4.25 (t, 2H), 6.15 (s, 1H), 6.9 (dd,
1H), 7.25 (s, 1H), 7.32 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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MS-EI : 134 [MH]⁺

¹H NMR λ[°] 710: (CDCl₃) 2.35 (s, 3H) ; 2.6 (t, 2H) ; 2.65 (t, 2H) ; 3.35 (s, 3H) ; 3.5 (t, 2H) ; 3.6 (t, 2H)

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¹H NMR λ[°] 710: (DMSOd₆) 1.9-2.1 (m, 2H), 2.4 (s, 3H), 2.45 (t, 2H), 2.45-2.6 (s, 4H), 3.6 (t, 4H), 4.0 (s, 3H), 4.25 (t, 2H), 6.15 (s, 1H), 6.9 (d, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.38 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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¹H NMR λ[°] 710: (DMSOd₆) 1.65-1.78(m, 2H); 2.50(t, 4H); 2.60(t, 2H); 3.68(t, 4H); 3.78(t, 2H); 4.90(br d, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 2.42 (s, 3H), 3.27 (s, 3H), 3.5 (t, 2H), 3.65 (t, 2H), 3.85 (t, 2H), 4.0 (s, 3H), 4.32 (t, 2H), 6.15 (s, 1H), 6.9 (d, 1H), 7.3 (s, 1H), 7.35 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 1.9-2.0 (m, 2H), 2.17 (s, 6H), 2.4 (s, 3H), 3.98 (s, 3H), 4.22 (t, 2H), 6.14 (s, 1H), 6.88 (dd, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.35 (s, 1H), 7.6 (s, 1H), 8.47 (s, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 1.9-2.0 (m, 2H), 2.38 (s, 3H), 2.65 (t, 2H), 2.9 (br s, 4H), 3.1 (br s, 4H), 3.96 (s, 3H), 4.25 (t, 2H), 6.12 (s, 1H), 6.85 (dd, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.37 (s, 1H), 7.56 (s, 1H), 8.46 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 2.42 (s, 3H), 3.96 (s, 3H), 4.62 (m, 2H), 4.75 (m, 2H), 6.15 (s, 1H), 6.9 (dd, 1H), 7.27 (s, 1H), 7.32 (d, 1H), 7.47 (s, 1H), 7.63 (s, 1H), 8.03 (s, 1H), 8.51 (s, 1H), 8.60 (s, 1H)

^1H NMR λ° H_2O : (DMSO- d_6) 2.15 (s, 3H), 2.2-2.6 (m, 10H), 2.4 (s, 3H), 3.65 (t, 2H), 3.85 (t, 2H), 4.03 (s, 3H), 4.35 (m, 2H), 6.16 (s, 1H), 6.9 (dd, 1H), 7.3 (s, 1H), 7.35 (d, 1H), 7.4 (s, 1H), 7.61 (s, 1H), 8.5 (s, 1H)

^1H NMR λ° H_2O : (DMSO- d_6) 2.40 (s, 3H), 2.4-2.5 (m, 4H), 2.4-2.6 (m, 2H), 3.55 (t, 4H), 3.6 (t, 2H), 3.85 (t, 2H), 3.97 (br s, 3H), 4.15 (br s, 2H), 6.15 (s, 1H), 6.9 (d, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.48 (s, 1H)

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MS - (EI): 175 [M.]⁺¹H NMR 300 MHz (CDCl₃) 2.5(br s, 4H); 2.59(t, 2H); 3.6-3.85(m, 10H)

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MS - ESI: 447 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.35-1.4 (m, 2H), 1.45-1.55 (m, 4H), 1.92-2.0 (m, 2H), 2.3-2.4 (m, 4H), 2.40 (s, 3H), 2.4-2.5 (m, 2H), 3.97 (s, 3H), 4.22 (t, 2H), 6.15 (s, 1H), 6.9 (d, 1H), 7.27 (s, 1H), 7.8 (d, 1H), 7.35 (s, 1H), 7.58 (s, 1H), 8.48 (s, 1H)

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MS - ESI: 427-429 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.12 (s, 9H), 2.32 (t, 2H), 3.7 (t, 2H), 3.9 (s, 3H), 4.25 (t, 2H), 5.9 (s, 2H), 7.20 (s, 1H), 7.51 (s, 1H), 8.36 (s, 1H)

元素分析 : 実測値 C 50.1 H 5.4 N 6.4

C₁₈H₂₃BrN₂O₅ · 0.2H₂O 理論値 C 50.2 H 5.5 N 6.5%

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MS - ESI: 432 [MH]⁺

¹H NMR 溶媒: (DMSO-d₆) 1.15 (s, 9H), 1.35-1.5 (m, 1H), 1.6-1.8 (m, 3H),
1.8-1.9 (d, 2H), 2.2-2.3 (m, 2H), 2.95 (t, 2H), 3.25 (t, 2H), 3.55 (d, 2H), 3.95 (s,
3H), 4.25 (t, 2H), 5.94 (s, 2H), 7.24 (s, 1H), 7.56 (s, 1H), 8.46 (s, 1H)

MS - ESI: 318 [MH]⁺

¹H NMR 溶媒: (DMSO-d₆) 1.3-1.4 (m, 2H), 1.4-1.55 (m, 4H), 1.85-1.95 (m,
2H), 2.35 (br s, 4H), 2.4 (t, 2H), 3.9 (s, 3H), 4.15 (t, 2H), 7.11 (s, 1H), 7.44 (s,
1H), 7.9 (s, 1H)

元素分析	:	実測値	C	63.5	H	7.4	N	13.1
C ₁₇ H ₂₃ N ₃ O ₃ · 0.2H ₂ O		理論値	C	63.6	H	7.4	N	13.0%

MS - ESI: 336 [MH]⁺

¹H NMR 溶媒: (DMSO-d₆) 1.35-1.45 (m, 2H), 1.5-1.6 (m, 4H), 1.9-2.05 (m, 2H), 2.4 (br s, 4H), 2.45 (t, 2H), 4.0 (s, 3H), 4.29 (t, 2H), 7.41 (s, 1H), 7.46 (s, 1H), 8.9 (s, 1H)

MS - ESI: 433 [MH]⁺

¹H NMR 溶媒: (DMSO-d₆) 1.4 (br s, 2H), 1.45-1.6 (br s, 4H), 1.9-2.1 (m, 2H), 2.4 (br s, 4H), 2.45 (t, 2H), 4.0 (s, 3H), 4.25 (t, 2H), 6.47 (s, 1H), 7.0 (d, 1H), 7.35 (s, 1H), 7.45 (s, 2H), 7.47 (d, 1H), 7.61 (s, 1H), 8.49 (s, 1H)

MS - ESI: 541 [MNa]⁺

¹H NMR 溶液: (DMSO-d₆) 1.1-1.3 (m, 2H), 1.4 (s, 9H), 1.8 (d, 2H), 1.95-2.1 (m, 1H), 2.4 (s, 1H), 2.7-2.85 (br s, 2H), 3.95 (s, 3H), 4.05 (d, 2H), 6.12 (s, 1H), 6.85 (d, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.35 (s, 1H), 7.55 (s, 1H), 8.45 (s, 1H)

MS - ESI: 419 [MH]⁺

¹H NMR 測定値: (DMSO-d₆, CF₃COOD) 1.5-1.7 (m, 2H), 2.05 (br d, 2H), 2.3-2.4 (m, 1H), 2.4 (s, 3H), 3.05 (t, 2H), 3.4 (d, 2H), 4.09 (s, 3H), 4.25 (d, 2H), 6.95 (dd, 1H), 7.35 (s, 1H), 7.4 (d, 1H), 7.6 (s, 1H), 7.85 (s, 1H), 9.15 (s, 1H)

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MS - ESI 477 [MH]⁺

¹H NMR 測定値: (DMSO-d₆, CF₃COOD) 1.6-1.8 (m, 2H), 2.05 (br d, 2H), 2.15-2.3 (m, 1H), 2.4 (s, 3H), 3.05 (t, 2H), 3.3 (br s, 2H), 3.32 (s, 3H), 3.58 (d, 2H), 3.65 (br s, 2H), 4.05 (s, 3H), 4.18 (d, 2H), 6.2 (s, 0.5 H (partly exchanged)), 6.92 (dd, 1H), 7.32 (s, 1H), 7.35 (d, 1H), 7.55 (s, 1H), 7.8 (s, 1H), 9.15 (s, 1H)

元素分析	:	実測値	C	68.0	H	6.8	N	11.8
C ₂₇ H ₃₂ N ₄ O ₄		理論値	C	68.1	H	6.8	N	11.8%

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MS - ESI: 472 [MH]⁺
¹H NMR (DMSO-d₆, CF₃COOD) 1.8-1.95 (m, 2H), 1.95-2.1 (m, 2H), 2.48 (s, 3H), 3.0-3.2 (m, 2H), 3.35 (t, 2H), 3.6 (t, 2H), 3.65 (br s, 2H), 4.11 (s, 3H), 6.18 (s, 0.5H, partially exchanged), 6.95 (dd, 1H), 7.05 (d, 1H), 7.35 (s, 1H), 7.37 (d, 1H), 7.8 (s, 1H), 7.86 (d, 1H), 8.2 (s, 1H), 8.76 (s, 1H)

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¹H NMR (400 MHz, DMSO-d₆) 4.15 (s, 3H), 7.5 (d, 1H), 7.62 (t, 1H), 7.78 (d, 1H), 8.02 (s, 1H), 8.27 (s, 1H), 8.77 (s, 1H)[illegible]

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MS - ESI: 431 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.51 (s, 9H), 4.07 (s, 3H), 6.87 (d, 1H), 7.45 (d, 1H), 7.6 (t, 1H), 7.7 (s, 1H), 7.75 (d, 1H), 7.91 (d, 1H), 8.39 (s, 1H), 8.65 (s, 1H)

元素分析	:	実測値	C	61.1	H	4.8	N	6.6
C ₂₂ H ₂₆ ClFN ₂ O ₃		理論値	C	61.3	H	4.7	N	6.5%

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¹H NMR 測定値: (DMSO-d₆) 4.08 (s, 3H), 6.9 (d, 1H), 7.45 (s, 1H), 7.6 (t, 1H), 7.70 (s, 1H), 7.73 (d, 1H), 7.95 (d, 1H), 8.39 (s, 1H), 8.66 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 2.4 (s, 3H), 4.06 (s, 3H), 6.15 (s, 1H), 6.82 (d, 1H), 6.9 (dd, 1H), 7.3 (s, 1H), 7.35 (d, 1H), 7.68 (s, 1H), 7.84 (d, 1H), 8.25 (s, 1H), 8.55 (s, 1H)

MS - ESI: 398 [MH] $^+$

^1H NMR λ° H_2O : (DMSO- d_6) 2.2-2.35 (m, 2H), 2.4 (s, 3H), 3.85 (t, 2H), 4.0 (s, 3H), 4.32 (t, 2H), 6.15 (s, 1H), 6.88 (d, 1H), 7.27 (s, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

MS - ESI: 462 [MH]⁺

¹H NMR 測定条件: (DMSO-d₆, CF₃COOD, 60°C) 2.2-2.3 (m, 2H), 2.4 (s, 3H),
2.9 (s, 3H), 3.4-3.5 (m, 4H), 3.5-3.8 (m, 6H), 4.07 (s, 3H), 4.4 (t, 2H), 6.95 (d,
1H), 7.35 (s, 1H), 7.4 (d, 1H), 7.55 (s, 1H), 7.8 (s, 1H), 8.95 (s, 1H)

MS - ESI 421 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.0 (t, 6H), 2.41 (s, 3H), 2.6 (q, 4H), 2.88 (t, 2H),
3.97 (s, 3H), 4.24 (t, 2H), 6.14 (s, 1H), 6.89 (dd, 1H), 7.25 (s, 1H), 7.32 (d, 1H),
7.38 (s, 1H), 7.58 (s, 1H), 8.48 (s, 1H)

元素分析	:	実測値	C	66.2	H	6.9	N	13.1
C ₂₄ H ₂₈ N ₄ O ₃ · 0.8H ₂ O		理論値	C	66.3	H	6.9	N	12.9%

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MS - ESI: 549 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.4 (s, 9H), 1.3-1.5 (m, 2H), 1.7-1.9 (m, 2H),
2.38 (s, 3H), 3.0 (br t, 2H), 3.5-3.7 (m, 3H), 3.85 (m, 2H), 3.98 (s, 3H), 4.3 (t,
2H), 6.12 (s, 1H), 6.85 (d, 1H), 7.22 (s, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.55 (s,
1H), 8.48 (s, 1H)

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¹H NMR スペクトル: (CDCl₃): 1.46 (s, 9H), 1.65 (t, 4H), 3.5 (t, 4H), 3.97 (s, 4H)

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MS - ESI: 268 [MNa]⁺

¹H NMR スペクトル: (CDCl₃) 1.48 (s, 9H), 1.5-1.6 (m, 2H), 1.8-1.9 (m, 2H), 2.0 (t, 1H), 3.05-3.15 (m, 2H), 3.5 (m, 1H), 3.57 (t, 2H), 3.7-3.9 (m, 4H)

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¹H NMR spectrum (DMSO-d₆): 1.2-1.4 (m, 2H), 1.8-1.9 (m, 2H), 2.47 (s, 3H), 2.4-2.5 (m, 2H), 2.9-3.0 (d, 2H), 3.3-3.5 (m, 1H), 3.95 (s, 2H), 4.0 (s, 3H), 4.35 (s, 2H), 6.15 (s, 1H), 6.9 (dd, 1H), 7.28 (s, 1H), 7.32 (d, 1H), 7.41 (s, 1H), 7.60 (s, 1H), 8.49 (s, 1H)
MS-ESI: 448 [M]⁺

¹H NMR spectrum (DMSO-d₆): 2.40 (s, 3H), 3.97 (s, 3H), 4.52 (t, 2H), 4.58 (t, 2H), 6.14 (s, 1H), 6.89 (dd, 1H), 7.07 (d, 2H), 7.26 (s, 1H), 7.31 (d, 1H), 7.46 (s, 1H), 7.61 (s, 1H), 8.41 (d, 2H), 8.5 (s, 1H)
MS-ESI: 443 [MH]⁺

元素分析	実測値	C	66.6	H	5.0	N	12.5
C ₂₅ H ₂₂ N ₄ O ₄ 0.12 CH ₂ Cl ₂	理論値	C	66.9	H	5.0	N	12.4%

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$^1\text{H NMR}$ λ° H_2O : (DMSO- d_6) 2.4 (s, 3H), 2.93 (s, 3H), 3.0 (s, 3H), 3.62 (t, 2H),
4.0 (s, 3H), 4.38 (t, 2H), 6.14 (s, 1H), 6.88 (dd, 1H), 7.26 (s, 1H), 7.3 (d, 1H),
7.43 (s, 1H), 7.61 (s, 1H), 8.49 (s, 1H)

MS-ESI : 457 $[\text{MH}]^+$

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^1H NMR スペクトル: (DMSO-d_6) 1.4-1.55 (m, 2H), 1.8-1.9 (m, 2H), 2.15 (t, 2H),
2.4 (s, 3H), 2.55 (t, 2H), 2.65 (t, 2H), 2.7-2.8 (m, 2H), 3.4-3.5 (m, 1H), 3.85 (m,
2H), 4.0 (s, 3H), 4.3 (t, 2H), 6.15 (s, 1H), 6.9 (dd, 1H), 7.25 (s, 1H), 7.3 (d, 1H),
7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

MS-ESI: 502 $[\text{MH}]^+$

元素分析	実測値	C	67.0	H	6.2	N	14.0
$\text{C}_{28}\text{H}_{31}\text{N}_5\text{O}_4$	理論値	C	67.1	H	6.2	N	14.0%

^1H NMR λ° C_6H_6 : (DMSO- d_6) 1.85 (br s, 4H), 2.15-2.25 (m, 2H), 2.85-3.15 (m, 6H), 4.01 (s, 3H), 4.32 (t, 2H), 6.5 (s, 1H), 6.95 (dd, 1H), 7.32 (s, 1H), 7.4 (s, 2H), 7.6 (d, 1H), 7.65 (s, 1H), 8.52 (s, 1H)

MS-ESI : 419 $[\text{MH}]^+$

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^1H NMR λ° C_6H_6 : (DMSO- d_6) 1.8-2.0 (m, 2H), 2.0-2.15 (m, 2H), 2.2-2.32 (m, 2H), 2.41 (s, 3H), 3.0-3.2 (m, 2H), 3.4 (t, 2H), 3.6-3.7 (m, 2H), 4.35 (t, 2H), 6.2 (s, 1H), 6.95 (dd, 1H), 7.3 (s, 1H), 7.35 (d, 1H), 7.5 (s, 1H), 7.57 (dd, 1H), 8.5 (d, 1H), 9.15 (s, 1H)

MS-ESI : 403 $[\text{MH}]^+$

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m.p. 267-269°C

^1H NMR スペクトル: (DMSO- d_6 ; CF₃COOD) 5.32(s, 2H); 7.25(d, 1H); 7.32-7.52(m, 6H); 8.12(d, 1H); 8.99(s, 1H)

MS - ESI: 252 [MH]⁺

元素分析	:	実測値	C	71.4	H	4.9	N	10.7
C ₁₅ H ₁₂ N ₂ O ₂ 0.04H ₂ O		理論値	C	71.2	H	4.8	N	11.1%

^1H NMR スペクトル: (DMSO- d_6) 5.4 (s, 2H); 7.35-7.65 (m, 6H); 8.2 (d, 1H); 9.0 (s, 1H)

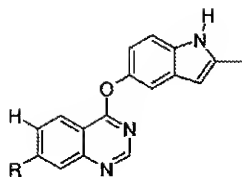
MS - ESI: 270 [MH]⁺

MS-ESI : 382 [MH]⁺

¹H NMR 300 MHz (DMSO-d₆) 2.41 (s, 3H), 5.4 (s, 2H), 6.15 (s, 1H), 6.9 (dd, 1H), 7.3 (s, 1H), 7.35 (d, 1H), 7.4 (d, 1H), 7.4-7.5 (m, 4H), 7.55 (d, 2H), 8.32 (d, 1H), 8.6 (s, 1H).

¹H NMR 300 MHz (DMSO-d₆) 2.4 (s, 3H), 6.14 (s, 1H), 6.88 (dd, 1H), 7.17 (s, 1H), 7.25-7.3 (m, 2H), 7.30 (d, 1H), 8.24 (d, 1H), 8.5 (s, 1H)

表 VI



実施例 番号	重量 (mg)	収量 %	MS-ESI [MH] ⁺	R	註
83	34	24	412		a
84	45	32	405		b
85	5	3	417		c
86	56	35	467		d
87	63	44	419		e
88	24	17	403		f
89	84	63	387		g

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^1H NMR スペクトル: (DMSO-d_6 , CF_3COOD) 2.2-2.3 (m, 2H), 2.4 (s, 3H), 3.05 (s, 3H), 3.3-3.45 (m, 2H), 4.4 (t, 2H), 6.2 (s, 1H), 6.95 (dd, 1H), 7.38 (s, 1H), 7.4 (d, 1H), 7.5 (s, 1H), 7.6 (dd, 1H), 8.5 (d, 1H), 9.2 (s, 1H)

元素分析	実測値	C	60.2	H	5.3	N	10.6
$\text{C}_{21}\text{H}_{21}\text{N}_3\text{O}_4\text{S}$ 0.4 DMF	理論値	C	60.5	H	5.4	N	10.8%

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^1H NMR スペクトル: (DMSO-d_6 , CF_3COOD) 2.4 (s, 3H), 3.1-3.3 (m, 2H), 3.62 (d, 2H), 3.7-3.9 (m, 4H), 4.05 (d, 2H), 4.7 (t, 2H), 6.2 (s, 0.5 H, partially exchanged), 6.95 (dd, 1H), 7.35 (s, 1H), 7.39 (d, 1H), 7.6 (s, 1H), 7.65 (dd, 1H), 8.55 (d, 1H), 9.15 (s, 1H)

元素分析	実測値	C	67.2	H	6.0	N	13.5
$\text{C}_{23}\text{H}_{24}\text{N}_4\text{O}_3$ 0.3 H_2O	理論値	C	67.4	H	6.1	N	13.7%

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^1H NMR スペクトル: (DMSO-d_6 , CF_3COOD) 1.2-1.5 (m, 2H), 1.6-1.8 (m, 2H), 1.8-1.9 (m, 2H), 2.25-2.35 (m, 2H), 2.45 (s, 3H), 2.95 (t, 2H), 3.25-3.3 (m, 2H), 3.55 (d, 2H), 4.4 (t, 2H), 6.95 (dd, 1H), 7.4 (s, 1H), 7.45 (d, 1H), 7.5 (s, 1H), 7.6 (d, 1H), 8.55 (d, 1H), 9.15 (s, 1H)

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^1H NMR スペクトル: (DMSO-d_6) 1.9-2.0 (m, 2H), 2.4 (s, 3H), 1.6-1.7 (m, 2H), 2.9 (br s, 4H), 3.1 (br s, 4H), 4.25 (t, 2H), 6.12 (s, 1H), 6.85 (d, 1H), 7.22 (s, 1H), 7.3 (d, 1H), 7.3-7.4 (m, 2H), 8.25 (d, 1H), 8.55 (s, 1H)

^1H NMR スペクトル: (DMSO-d_6) 1.95-2.05 (m, 2H), 2.42 (s, 3H), 2.5 (t, 2H), 2.55 (t, 4H), 3.6 (t, 4H), 4.3 (t, 2H), 6.18 (s, 1H), 6.9 (dd, 1H), 7.3 (s, 1H), 7.35 (d, 1H), 7.3-7.4 (m, 2H), 8.3 (d, 1H), 8.6 (s, 1H)

元素分析

実測値

C 66.5

H 6.2

N 12.7

$\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_3 \cdot 0.14 \text{CH}_2\text{Cl}_2 \cdot 0.7 \text{H}_2\text{O}$

理論値

C 66.7

H 6.4

N 13.0%

^1H NMR スペクトル: (DMSO-d_6) 1.4-1.5 (br s, 2H), 1.5-1.7 (br s, 4H), 2.42 (s, 3H),
2.5-2.7 (br s, 4H), 2.8-3.0 (br s, 2H), 4.35 (br s, 2H), 6.18 (s, 1H), 6.9 (dd, 1H),
7.3 (s, 1H), 7.35 (d, 1H), 7.4 (d, 1H), 7.42 (s, 1H), 8.3 (d, 1H), 8.6 (s, 1H)

元素分析	実測値	C	69.0	H	6.6	N	13.4
$\text{C}_{26}\text{H}_{26}\text{N}_4\text{O}_2 \cdot 0.8 \text{H}_2\text{O}$	理論値	C	69.1	H	6.7	N	13.4%

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^1H NMR スペクトル: (DMSO-d_6) 2.4 (s, 3H), 4.6 (m, 2H), 4.7 (m, 2H), 6.15 (s,
1H), 6.9 (dd, 1H), 7.28 (s, 1H), 7.3 (d, 2H), 7.4 (s, 1H), 8.02 (s, 1H), 8.3 (d,
1H), 8.6 (s, 1H), 8.65 (s, 1H)

元素分析	実測値	C	63.7	H	4.8	N	21.5
$\text{C}_{21}\text{H}_{18}\text{N}_6\text{O}_2 \cdot 0.5 \text{H}_2\text{O}$	理論値	C	63.8	H	4.8	N	21.3%

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^1H NMR スペクトル: (DMSO-d_6) 1.3-1.4 (m, 2H), 1.42 (s, 9H), 1.85 (d, 2H), 2.0-2.1 (m, 1H), 2.42 (s, 3H), 2.7-2.9 (br s, 2H), 3.95-4.05 (m, 2H), 4.1 (d, 2H), 6.15 (s, 1H), 6.9 (dd, 1H), 7.3 (s, 1H), 7.33 (d, 1H), 7.38 (s, 1H), 7.35-7.4 (m, 1H), 8.3 (d, 1H), 8.6 (s, 1H)

MS-ESI: 489 $[\text{MH}]^+$

元素分析	実測値	C	68.7	H	6.7	N	11.3
$\text{C}_{28}\text{H}_{32}\text{N}_4\text{O}_4$	理論値	C	68.8	H	6.6	N	11.5%

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^1H NMR スペクトル: (DMSO-d_6) 1.6-1.75 (m, 4H), 2.12 (s, 3H), 2.28 (s, 3H), 2.52 (br s, 4H), 3.85 (t, 2H), 3.93 (s, 3H), 4.25 (t, 2H), 6.8 (d, 1H), 7.17 (s, 1H), 7.22 (d, 1H), 7.33 (s, 1H), 7.54 (s, 1H), 8.43 (s, 1H)

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¹H NMR スペクトル: (DMSO-d₆) 2.1 (s, 3H); 2.3 (s, 3H); 6.5 (dd, 1H); 6.65 (d, 1H); 7.0 (d, 1H); 8.45 (s, 1H)

¹H NMR (λ^o 400 MHz; (DMSO-d₆) 2.15 (s, 3H); 2.35 (s, 3H); 4.02 (s, 3H); 5.4 (s, 2H); 6.9 (dd, 1H); 7.22 (d, 1H); 7.3 (d, 1H); 7.35-7.6 (m, 6H); 7.65 (s, 1H); 8.5 (s, 1H)

[illegible]

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^1H NMR スペクトル: ($\text{DMSO}-d_6$) 2.1 (s, 3H); 2.32 (s, 3H); 3.97 (s, 3H); 7.85 (dd, 1H); 7.2 (bs, 2H); 7.25 (d, 1H); 7.58 (s, 1H); 8.4 (s, 1H)

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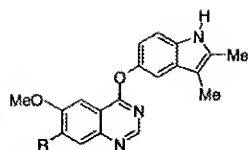
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表 VII



実施例 番号	重量 (mg)	収量 %	MS-ESI [MH] ⁺	R	HPLC* RT (min)	註
92	91	65	431		-	a
93	78	55	438		-	b
94	34	27	435		-	c
95	39	33	407		-	d
96	58	44	449		-	e
97	58	47	421		-	f
98	85	66	447		-	g
99	24	18	447		-	h
100	110	82	461		-	i
101	9	7	447		-	j
102	81	62	463		3.4	k
103	75	57	451		-	l
104	96	65	511		-	m
105	103	78	457		-	n
106	64	49	456		-	o

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¹H NMR ｽﾍﾞｸﾄﾙ: (DMSO-d₆) 2.10 (s, 3H), 2.30 (s, 3H), 3.93 (s, 3H), 4.52 (m, 2H), 4.55-4.65 (m, 2H), 6.85 (d, 1H), 7.2 (s, 1H), 7.25 (d, 1H), 7.4 (d, 1H), 7.58 (s, 1H), 8.0 (s, 1H), 8.48 (s, 1H), 8.58 (s, 1H)

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¹H NMR ｽﾍﾞｸﾄﾙ: (DMSO-d₆) 2.14 (s, 3H), 2.35 (s, 3H), 3.3 (s, 3H), 3.5 (t, 2H), 3.65 (t, 2H), 3.85 (t, 2H), 4.0 (s, 3H), 4.32 (t, 2H), 6.9 (d, 1H), 7.25 (d, 1H), 7.28 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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¹H NMR ｽﾍﾞｸﾄﾙ: (DMSO-d₆) 1.05 (t, 6H), 2.15 (s, 3H), 2.35 (s, 3H), 2.6-2.7 (m, 4H), 2.92 (br s, 2H), 4.0 (s, 3H), 4.25 (t, 2H), 6.9 (dd, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

¹H NMR spectrum (DMSO-d₆): 2.15 (s, 3H), 2.35 (s, 9H), 2.85 (br s, 2H), 4.0 (s, 3H), 4.35 (t, 2H), 6.87 (dd, 1H), 7.22 (s, 1H), 7.3 (d, 1H), 7.42 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

¹H NMR spectrum (DMSO-d₆): 2.15 (s, 3H), 2.35 (s, 3H), 3.25-3.4 (m, 2H), 3.65 (d, 2H), 3.7-3.8 (m, 4H), 4.0-4.1 (m, 2H), 4.1 (s, 3H), 4.7 (t, 2H), 6.95 (dd, 1H), 7.3 (s, 1H), 7.35 (d, 1H), 7.6 (s, 1H), 7.8 (s, 1H), 9.0 (s, 1H)

¹H NMR spectrum (DMSO-d₆): 1.95-2.05 (m, 2H), 2.15 (s, 3H), 2.2 (s, 6H), 2.35 (s, 3H), 2.45 (t, 2H), 4.0 (s, 3H), 4.25 (t, 2H), 6.9 (dd, 1H), 7.22 (d, 1H), 7.3 (d, 1H), 7.37 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 1.9-2.05 (m, 4H), 2.15 (s, 3H), 2.25 (t, 2H), 2.35 (s, 3H), 3.65 (t, 2H), 4.0 (s, 3H), 4.35 (t, 2H), 6.9 (d, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.45 (s, 1H), 7.62 (s, 1H), 8.5 (s, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 1.0-1.15 (m, 1H), 1.25-1.4 (m, 2H), 1.5 (br s, 1H), 1.65 (d, 1H), 1.7-1.8 (m, 1H), 1.8-1.9 (m, 2H), 2.15 (s, 3H), 2.35 (s, 3H), 2.5 (d, 1H), 2.6-2.7 (m, 1H), 2.9-3.0 (m, 1H), 4.0 (s, 3H), 4.2-4.35 (m, 2H), 6.88 (dd, 1H), 7.2 (s, 1H), 7.27 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 2.12 (s, 3H), 2.35 (s, 3H), 2.68 (s, 4H), 3.85 (t, 2H), 3.95 (s, 3H), 4.35 (t, 2H), 6.88 (dd, 1H), 7.22 (s, 1H), 7.25 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

^1H NMR λ° H_2O : (DMSO-d_6) 1.95-2.05 (m, 2H), 2.15 (s, 3H), 2.35 (s, 3H), 2.42 (br s, 4H), 2.5 (t, 2H), 3.6 (m, 4H), 4.0 (s, 3H), 4.25 (t, 2H), 6.85 (dd, 1H), 7.25 (d, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H).

^1H NMR λ° H_2O : (DMSO-d_6) 2.15 (s, 3H), 2.35 (s, 6H), 2.65 (t, 2H), 2.9 (t, 2H), 3.25 (s, 3H), 3.45 (t, 2H), 4.0 (s, 3H), 4.3 (t, 2H), 6.9 (dd, 1H), 7.22 (s, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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^1H NMR λ° g t : (DMSO- d_6) 1.95-2.05 (m, 2H), 2.15 (s, 3H), 2.35 (s, 3H), 2.7 (t, 2H), 2.95 (br s, 4H), 3.15 (br s, 4H), 4.0 (s, 3H), 4.29 (t, 2H), 6.9 (dd, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.61 (s, 1H), 8.5 (s, 1H)

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^1H NMR λ° g t : (DMSO- d_6) 2.15 (s, 3H), 2.35 (s, 3H), 4.0 (s, 3H), 4.55 (m, 2H), 4.6 (m, 2H), 6.88 (dd, 1H), 7.08 (d, 2H), 7.22 (s, 1H), 7.28 (d, 1H), 7.48 (s, 1H), 7.6 (s, 1H), 8.42 (d, 2H), 8.5 (s, 1H), 10.78 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 1.8-1.9 (m, 2H), 2.15 (s, 3H), 2.25-2.35 (m, 2H),
2.35 (s, 3H), 3.0 (s, 3H), 4.02 (s, 3H), 4.35 (t, 2H), 6.9 (dd, 1H), 7.25 (s, 1H),
7.3 (d, 1H), 7.4 (s, 1H), 7.7 (s, 1H), 8.52 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 3.3 (s, 3H), 3.5 (m, 2H), 3.65 (m, 2H), 3.85 (m,
2H), 4.02 (s, 3H), 4.35 (t, 2H), 6.58 (s, 1H), 7.0 (dd, 1H), 7.4 (s, 1H), 7.45 (br s,
2H), 7.47 (d, 1H), 7.61 (s, 1H), 8.5 (s, 1H)

MS-ESI : 410 [MH] $^+$

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^1H NMR λ^{\wedge} Ct Ct : (DMSO-d_6) 4.02 (s, 3H), 5.4 (s, 2H), 6.5 (s, 1H), 7.0 (dd, 1H),
7.4-7.6 (m, 9H), 7.65 (s, 1H), 8.5 (s, 1H), 11.23 (s, 1H)
MS-ESI : 398 [MH] $^{+}$

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^1H NMR λ^{\wedge} Ct Ct : (DMSO-d_6) 4.0 (s, 3H), 6.46 (s, 1H), 7.01 (dd, 1H), 7.2 (s,
1H), 7.4-7.5 (m, 3H), 7.6 (s, 1H), 8.41 (s, 1H)

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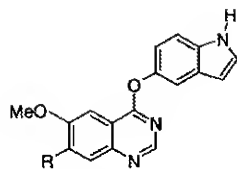
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表 VIII



実施例 番号	重量 (mg)	収量 %	MS-ESI [MH] ⁺	R	註
108	58	49	407		r
109	14	13	379		s
110	55	48	393		t
111	27	23	405		u
112	58	47	421		v
113	63	52	419		w
114	64	53	419		x
115	106	84	435		y
116	76	62	423		z
117	113	81	483		aa
118	24	19	429		bb

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^1H NMR スペクトル: (DMSO-d_6) 2.3 (s, 6H), 2.8 (t, 2H), 4.0 (s, 3H), 4.3 (t, 2H),
6.45 (s, 1H), 7.0 (dd, 1H), 7.4-7.5 (m, 4H), 7.6 (s, 1H), 8.5 (s, 1H)

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^1H NMR スペクトル: (DMSO-d_6) 1.9-2.05 (m, 2H), 2.21 (s, 6H), 2.45 (t, 2H), 4.02
(s, 3H), 4.25 (t, 2H), 6.47 (s, 1H), 7.0 (dd, 1H), 7.38 (s, 1H), 7.35-7.4 (m, 2H),
7.45 (d, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

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^1H NMR λ^\wedge H : (DMSO- d_6) 0.95 (t, 6H), 1.9-2.0 (m, 2H), 2.5 (m, 4H), 2.6 (t, 2H), 4.0 (s, 3H), 4.25 (t, 2H), 6.48 (s, 1H), 7.0 (dd, 1H), 7.38 (s, 1H), 7.42-7.5 (m, 3H), 7.6 (s, 1H), 8.5 (s, 1H)

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^1H NMR λ^\wedge H : (DMSO- d_6) 1.45-1.75 (m, 3H), 1.75-1.85 (m, 2H), 2.0-2.1 (m, 1H), 2.1-2.2 (m, 1H), 2.25-2.35 (m, 1H), 2.95 (t, 1H), 3.3-3.4 (m, 2H), 4.1 (s, 3H), 4.4-4.5 (m, 2H), 6.5 (s, 1H), 7.05 (dd, 1H), 7.45-7.6 (m, 4H), 7.75 (s, 1H), 9.0 (s, 1H)

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^1H NMR λ^\wedge H : (DMSO- d_6) 1.1-1.3 (m, 1H), 1.35-1.5 (m, 1H), 1.65-1.8 (m, 2H), 1.8-1.9 (m, 2H), 3.1 (t, 2H), 3.6 (d, 2H), 3.65 (t, 2H), 4.1 (s, 3H), 4.7 (t, 2H), 6.5 (d, 1H), 7.05 (dd, 1H), 7.45 (s, 1H), 7.5-7.55 (m, 2H), 7.61 (s, 1H), 7.8 (s, 1H), 9.0 (m, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 1.9-2.1 (m, 2H), 2.4 (br s, 4H), 2.5 (t, 2H), 3.6 (t, 4H), 4.0 (s, 3H), 4.25 (t, 2H), 6.45 (s, 1H), 7.0 (dd, 1H), 7.4 (s, 1H), 7.4-7.5 (m, 2H), 7.47 (d, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

^1H NMR λ° H_2O : (DMSO- d_6) 2.35 (s, 3H), 2.65 (t, 2H), 2.9 (t, 2H), 3.25 (s, 3H), 3.45 (t, 2H), 4.0 (s, 3H), 4.3 (t, 2H), 6.45 (s, 1H), 7.05 (dd, 1H), 7.4-7.5 (m, 4H), 7.6 (s, 1H), 8.5 (s, 1H)

^1H NMR λ° H_2O : (DMSO- d_6) 2.0 (m, 2H), 2.65 (m, 2H), 2.9 (br s, 4H), 3.15 (br s, 4H), 4.0 (s, 3H), 4.25 (t, 2H), 6.5 (s, 1H), 7.0 (dd, 1H), 7.35-7.5 (m, 4H), 7.65 (s, 1H), 8.5 (s, 1H)

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^1H NMR スペクトル: (DMSO-d_6) 1.35-1.45 (m, 2H), 1.45-1.55 (m, 4H), 1.9-2.05 (m, 2H), 2.3-2.4 (m, 4H), 2.45 (t, 2H), 4.0 (s, 3H), 4.22 (t, 2H), 6.5 (s, 1H), 6.9 (dd, 1H), 7.3 (s, 1H), 7.35-7.40 (m, 2H), 7.55-7.65 (m, 2H), 8.5 (s, 1H)

MS-ESI: 433 $[\text{MH}]^+$

元素分析	実測値	C	68.4	H	6.4	N	12.8
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_3 \cdot 0.4 \text{H}_2\text{O}$	理論値	C	68.3	H	6.6	N	12.7%

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^1H NMR λ° f° (DMSO- d_6) 2.2-2.35 (m, 2H), 3.05 (s, 3H), 3.3 (m, 2H), 4.0 (s, 3H), 4.35 (t, 2H), 6.48 (s, 1H), 6.9 (dd, 1H), 7.3 (s, 1H), 7.4 (2s, 2H), 7.6 (d, 1H), 7.65 (s, 1H), 7.9 (s, 1H)

MS-ESI : 428 [MH] $^+$

元素分析	実測値	C	56.2	H	4.9	N	9.3
$\text{C}_{21}\text{H}_{21}\text{N}_3\text{O}_5\text{S} \cdot 1.1 \text{H}_2\text{O}$	理論値	C	56.4	H	5.2	N	9.4%

^1H NMR λ° f° (DMSO- d_6) 1.95-2.05 (m, 2H), 2.4 (br s, 4H), 2.48 (t, 2H), 3.6 (t, 4H), 4.0 (s, 3H), 4.27 (t, 2H), 6.5 (s, 1H), 6.93 (dd, 1H), 7.3 (s, 1H), 7.4 (br s, 2H), 7.6 (d, 1H), 7.61 (s, 1H), 8.5 (s, 1H)

MS-ESI : 435 [MH] $^+$

元素分析	実測値	C	62.0	H	6.2	N	12.1
$\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_4 \cdot 1.6 \text{H}_2\text{O}$	理論値	C	62.2	H	6.4	N	12.1%

^1H NMR 測定値: (DMSO-d_6 , CF_3COOD) 1.5-1.65 (m, 2H), 2.0 (d, 2H), 2.15-2.3 (m, 1H), 2.4 (s, 3H), 2.95 (t, 2H), 3.38 (d, 2H), 4.2 (d, 2H), 6.2 (s, 0.5H, partially exchanged), 6.9 (dd, 1H), 7.35 (s, 1H), 7.4 (d, 1H), 7.5 (s, 1H), 7.58 (dd, 1H), 8.5 (d, 1H), 9.1 (s, 1H)

MS-ESI: 389 $[\text{MH}]^+$

元素分析

実測値 C 68.9 H 6.2 N 13.7

$\text{C}_{23}\text{H}_{24}\text{N}_4\text{O}_2 \cdot 0.2 \text{H}_2\text{O} \cdot 0.12 \text{CH}_2\text{Cl}_2$

理論値 C 69.0 H 6.2 N 13.9%

^1H NMR スペクトル: (DMSO-d_6) 1.3-1.42 (m, 2H), 1.7-1.9 (m, 3H), 2.0 (t, 2H), 2.4 (s, 3H), 2.48 (t, 2H), 2.92 (d, 2H), 3.22 (s, 3H), 3.42 (t, 2H), 4.05 (d, 2H), 6.15 (s, 1H), 6.88 (dd, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.35 (s, 1H), 7.37 (d, 1H), 8.28 (d, 1H), 8.6 (s, 1H)

MS-ESI: 447 $[\text{MH}]^+$

元素分析	実測値	C	68.4	H	6.7	N	12.2
$\text{C}_{26}\text{H}_{30}\text{N}_4\text{O}_3 \cdot 0.5 \text{H}_2\text{O}$	理論値	C	68.6	H	6.9	N	12.3%

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^1H NMR スペクトル: (DMSO-d_6) 1.25 (t, 3H), 2.2-2.3 (m, 2H), 2.4 (s, 3H), 3.2 (q, 2H), 3.3 (t, 2H), 4.0 (s, 3H), 4.35 (t, 2H), 6.15 (s, 1H), 6.9 (dd, 1H), 7.28 (s, 1H), 7.32 (d, 1H), 7.4 (s, 1H), 7.62 (s, 1H), 8.5 (s, 1H)

MS-ESI: 456 $[\text{MH}]^+$

元素分析	実測値	C	60.3	H	5.6	N	9.2
$\text{C}_{23}\text{H}_{25}\text{N}_3\text{O}_5\text{S}$	理論値	C	60.6	H	5.5	N	9.2%

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^1H NMR 測定値: (DMSO-d_6) 1.25 (t, 3H), 1.75-1.9 (m, 2H), 3.0-3.2 (m, 4H),
3.5 (q, 2H), 4.7 (t, 1H)
MS-ESI: 153 $[\text{MH}]^+$

^1H NMR 測定値: (DMSO-d_6) 1.25 (t, 3H), 2.15 (s, 3H), 2.2-2.3 (m, 2H), 2.35
(s, 3H), 3.2 (q, 2H), 3.3 (t, 2H), 4.02 (s, 3H), 4.35 (t, 2H), 6.9 (dd, 1H), 7.22 (s,
1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.63 (s, 1H), 8.51 (s, 1H)
MS-ESI: 470 $[\text{MH}]^+$

元素分析	実測値	C	60.6	H	6.0	N	8.8
$\text{C}_{24}\text{H}_{27}\text{N}_3\text{O}_5\text{S} \cdot 0.4 \text{H}_2\text{O}$	理論値	C	60.5	H	5.9	N	8.8%

[illegible]

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MS-ESI : 533 [MH]⁺

元素分析	実測値	C 67.8	H 6.9	N 10.5
$C_{30}H_{36}N_4O_5$	理論値	C 67.7	H 6.8	N 10.5%

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[illegible]

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^1H NMR スペクトル: (DMSO-d_6 , CF_3COOD) 1.3-1.5 (m, 4H), 1.6-1.7 (m, 1H),
1.7-1.9 (d, 2H), 1.75 (t, 2H), 3.25 (d, 2H), 3.55 (t, 2H)

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^1H NMR スペクトル: (DMSO-d_6) 0.9-1.1 (m, 2H), 1.3-1.6 (m, 3H), 1.4 (s, 9H), 1.6
(d, 2H), 2.5-2.8 (br s, 2H), 3.45 (dd, 2H), 3.9 (d, 2H), 4.35 (t, 1H)

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^1H NMR λ° f f : (DMSO-d_6 , CF_3COOD) 2.25-2.35 (m, 2H), 2.38 (s, 3H), 3.15 (t, 2H), 3.35 (t, 2H), 3.5 (d, 2H), 3.68 (t, 2H), 4.0 (d, 2H), 4.05 (s, 3H), 4.35 (t, 2H), 6.18 (s, 1H), 6.9 (d, 1H), 7.22 (s, 1H), 7.45 (d, 1H), 7.52 (s, 1H), 7.8 (s, 1H), 9.05 (s, 1H)

MS-ESI: 449 $[\text{MH}]^+$

元素分析	実測値	C	66.4	H	6.4	N	12.4
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_4 \cdot 0.2 \text{H}_2\text{O}$	理論値	C	66.4	H	6.3	N	12.4%

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^1H NMR λ° f f : (DMSO-d_6 , CF_3COOD) 1.3-1.5 (m, 2H), 1.8-2.0 (m, 5H), 2.4 (s, 3H), 2.9 (t, 2H), 3.3 (d, 2H), 4.05 (s, 3H), 4.35 (t, 2H), 6.2 (s, 1H), 6.95 (dd, 1H), 7.35 (s, 1H), 7.37 (d, 1H), 7.52 (s, 1H), 7.8 (s, 1H), 9.1 (s, 1H)

MS-ESI: 433 $[\text{MH}]^+$

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[illegible]¹H NMR スペクトル: (CDCl₃) 1.68(t, 1H); 4.18(d, 2H); 4.33(d, 2H)

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^1H NMR スペクトル: (CDCl_3) 1.82(t, 4H); 2.63(t, 4H); 3.44(t, 2H), 4.29(t, 2H)

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^1H NMR スペクトル: (CDCl_3) 1.82(m, 4H); 2.61(m, 4H); 3.17(m, 2H); 4.13(s, 2H); 5.84(m, 2H)

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^1H NMR λ^{\wedge} DMSO-d_6 : 2.16 (s, 3H), 2.33 (s, 3H), 4.0 (s, 3H), 5.34 (s, 2H), 7.2 (d, 1H), 7.32 (d, 1H), 7.35-7.55 (m, 7H), 8.2 (s, 1H), 8.7 (s, 1H), 10.9 (s, 1H), 11.15 (s, 1H)
MS-ESI: 425 [MH] $^{+}$

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^1H NMR λ° C_6H_6 : (DMSO-d_6) 2.2 (s, 3H), 2.35 (s, 3H), 3.97 (s, 3H), 7.0 (s, 1H),
7.22 (d, 1H), 7.3 (d, 1H), 7.55 (s, 1H), 7.85 (s, 1H), 8.28 (s, 1H), 9.35 (s, 1H),
10.2 (br s, 1H), 10.62 (s, 1H)
MS-ESI : 335 $[\text{MH}]^+$

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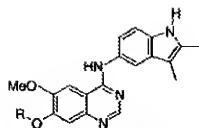
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表 IX



実施例 番号	重量 (mg)	収量%	MS-ESI [MH] ⁺	R	註
130	10	11	458		a
131	63	69	450		b
132	5	6	443		c
133	35	36	475		d
134	53	51	510		e
135	56	58	469		f
136	4	4.6	415		g
137	29	35	406		h
138	49	56	432		i
139	8	8.6	481		j
140	15	15	477		k
141	38	42	446		l
142	69	72	470		m
143	21	21	492		n
144	36	40	440		o
145	31	33	460		p

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¹H NMR 溶液 (CDCl₃): 2.12 (m, 2H) ; 2.6 (br s, 1H) ; 3.65 (t, 2H) ; 4.35 (t, 2H) ; 7.95 (s, 1H) ; 8.1 (s, 1H)

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MS-EI : 242 [MH]⁺¹H NMR 溶液: (CDCl₃) 0.25 (s, 6H) ; 0.9 (s, 9H) ; 2.05 (m, 2H) ; 3.52 (t, 2H) ; 4.25 (t, 2H) ; 7.9 (s, 1H) ; 8.02 (s, 1H)

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MS-EI : 256 [MH]⁺¹H NMR 溶液: (CDCl₃) 0.25 (s, 6H) ; 0.85 (s, 9H) ; 2.0 (t, 2H) ; 2.4 (s, 3H) ; 3.52 (t, 2H) ; 4.15 (t, 2H) ; 7.72 (s, 1H)

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MS-ESI : 142 [MH]⁺

¹H NMR 測定条件: (CDCl₃) 2.05 (m, 2H) ; 2.5 (s, 3H) ; 3.62 (t, 2H) ; 4.25 (t, 2H) ; 7.8 (s, 1H)

¹H NMR 測定条件: (DMSO-d₆) 2.15 (s, 3H), 2.35 (s, 6H), 2.65 (t, 2H), 2.85 (t, 2H), 3.25 (s, 3H), 3.45 (t, 2H), 3.95 (s, 3H), 4.2 (t, 2H), 7.15 (s, 1H), 7.22 (s, 1H), 7.3 (dd, 1H), 7.55 (s, 1H), 7.85 (s, 1H), 8.3 (s, 1H), 9.4 (s, 1H), 10.62 (s, 1H)

^1H NMR λ° C_6H_5 : (DMSO-d_6) 2.15 (s, 3H), 2.32 (s, 3H), 3.2 (t, 2H), 3.7 (s, 3H),
3.95 (s, 3H), 4.45 (t, 2H), 6.8 (s, 1H), 7.05 (s, 1H), 7.15 (s, 1H), 7.22 (d, 1H),
7.3 (dd, 1H), 7.55 (s, 1H), 7.88 (s, 1H), 8.32 (s, 1H), 9.4 (s, 1H), 10.62 (s, 1H)

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^1H NMR λ° C_6H_5 : (DMSO-d_6) 1.9-2.0 (m, 2H), 2.15 (2s, 6H), 2.0-2.9 (m, 8H),
2.32 (s, 3H), 2.45 (t, 2H), 3.95 (s, 3H), 4.2 (t, 2H), 7.1 (s, 1H), 7.22 (d, 1H), 7.3
(dd, 1H), 7.55 (s, 1H), 7.85 (s, 1H), 8.3 (s, 1H), 9.4 (s, 1H), 10.62 (s, 1H)

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^1H NMR λ° C_6H_5 : (CDCl_3) 1.72 (m, 2H) ; 2.3 (s, 3H) ; 2.2-2.8 (m, 8H) ; 2.6 (t,
2H) ; 3.8 (t, 2H) ; 5.3 (br s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 1.9-2.0 (m, 2H), 2.5 (s, 9H), 2.65 (t, 2H), 2.9 (br s, 4H), 3.15 (br s, 4H), 3.95 (s, 3H), 4.25 (t, 2H), 7.2 (s, 1H), 7.85 (s, 1H), 8.0 (dd, 1H), 8.15 (d, 1H), 8.2 (s, 1H), 8.45 (s, 1H), 9.6 (s, 1H), 10.95 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 2.15 (s, 3H), 2.35 (s, 3H), 3.07 (s, 3H), 3.85 (t, 2H), 3.95 (s, 3H), 4.3 (t, 2H), 6.7 (d, 2H), 7.15 (s, 1H), 7.22 (d, 1H), 7.3 (dd, 1H), 7.55 (s, 1H), 7.85 (s, 1H), 8.15 (d, 2H), 8.3 (s, 1H), 9.4 (s, 1H), 10.65 (s, 1H)

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¹H NMR (CDCl₃): 2.15 (s, 3H), 2.25 (s, 6H), 2.32 (s, 3H), 2.72 (t, 2H), 3.95 (s, 3H), 4.2 (t, 2H), 7.15 (s, 1H), 7.22 (d, 1H), 7.3 (dd, 1H), 7.55 (s, 1H), 7.85 (s, 1H), 8.32 (s, 1H), 9.4 (s, 1H), 10.6 (s, 1H)

¹H NMR スペクトル: (DMSO-d₆) 1.65-1.75 (m, 4H), 2.15 (s, 3H), 2.35 (s, 3H), 2.55-2.65 (m, 4H), 2.9 (t, 2H), 3.95 (s, 3H), 4.25 (t, 2H), 7.15 (s, 1H), 7.22 (d, 1H), 7.3 (dd, 1H), 7.55 (s, 1H), 7.85 (s, 1H), 8.32 (s, 1H), 9.4 (s, 1H), 10.62 (s, 1H)

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^1H NMR λ° DMSO-d_6 : 0.7 (s, 3H), 1.15 (s, 3H), 2.05-2.1 (m, 2H), 2.1 (s, 3H), 2.6 (s, 3H), 3.42 (d, 2H), 3.57 (d, 2H), 4.0 (s, 3H), 4.22 (t, 2H), 4.7 (t, 1H), 7.2 (s, 1H), 7.82 (s, 1H), 8.0 (dd, 1H), 8.17 (d, 1H), 8.3 (s, 1H), 8.45 (s, 1H), 9.6 (s, 1H), 10.95 (s, 1H)

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^1H NMR λ° DMSO-d_6 : 1.3-1.45 (m, 2H), 1.45-1.6 (m, 4H), 2.15 (s, 3H), 2.35 (s, 3H), 2.45 (br s, 4H), 2.75 (t, 2H), 3.95 (s, 3H), 4.25 (t, 2H), 7.15 (s, 1H), 7.22 (d, 1H), 7.3 (dd, 1H), 7.55 (s, 1H), 7.85 (s, 1H), 8.3 (s, 1H), 9.4 (s, 1H), 10.62 (s, 1H)

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^1H NMR λ° H_2O (DMSO- d_6) 2.15 (s, 3H), 2.32 (s, 3H), 3.1 (s, 3H), 3.9 (s, 3H),
3.95 (t, 2H), 4.35 (t, 2H), 6.85 (dd, 1H), 7.15 (s, 1H), 7.20 (d, 1H), 7.28 (dd,
1H), 7.55 (s, 1H), 7.85 (s, 1H), 8.3 (s, 1H), 8.58 (d, 1H), 8.9 (d, 1H), 9.4 (s,
1H), 10.62 (s, 1H)

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^1H NMR λ° H_2O (CDCl $_3$) 2.1(br s, 1H); 3.09(s, 3H); 3.71(t, 2H); 3.93(t, 2H);
6.8(s, 1H)
MS - ESI: 221 [MH] $^+$

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8.48(d, 1H); 8.54 (d, 1H)

MS - ESI: 153 [MH]⁺

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2.45-2.5 (m, 2H), 3.5-3.55 (m, 4H), 3.65 (t, 2H), 3.8-3.85 (m, 2H), 3.95 (s, 1H),

8.3 (s, 1H), 9.4 (s, 1H), 10.62 (s, 1H)

^1H NMR λ° CDCl_3 : 2.5(br s, 4H); 2.59(t, 2H); 3.6-3.85(m, 10H)
MS - (EI): 175 $[\text{M}]^+$

^1H NMR λ° DMSO-d_6 : 2.15 (s, 3H), 2.32 (s, 3H), 3.15 (t, 2H), 3.95 (s, 3H), 4.4 (t, 2H), 7.2 (s, 1H), 7.22 (d, 1H), 7.3 (dd, 1H), 7.35 (dd, 1H), 7.55 (s, 1H), 7.8 (d, 1H), 7.85 (s, 1H), 8.32 (s, 1H), 8.45 (dd, 1H), 8.6 (s, 1H), 9.4 (s, 1H), 10.68 (s, 1H)

^1H NMR λ° DMSO-d_6 : 1.9-2.05 (m, 4H), 2.12 (s, 3H), 2.15-2.3 (m, 2H), 2.6 (s, 3H), 3.3-3.45 (m, 4H), 4.0 (s, 3H), 4.15 (t, 2H), 7.15 (s, 1H), 7.82 (s, 1H), 8.0 (dd, 1H), 8.17 (d, 1H), 8.3 (s, 1H), 8.45 (s, 1H), 9.6 (s, 1H), 10.95 (s, 1H)

^1H NMR λ° DMSO-d_6 : 1.65-1.8 (m, 4H), 1.95-2.05 (m, 2H), 2.42 (s, 3H), 2.5 (br s, 1H), 2.6 (t, 2H), 4.0 (s, 3H), 4.27 (t, 2H), 6.2 (s, 1H), 6.85 (dd, 1H), 7.2 (s, 1H), 7.4 (s, 1H), 7.45 (d, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

MS-ESI: 433 $[\text{MH}]^+$

元素分析	実測値	C	68.3	H	6.4	N	12.8
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_3 \cdot 0.4 \text{H}_2\text{O}$	理論値	C	68.3	H	6.6	N	12.7%

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^1H NMR スペクトル: (DMSO-d_6) 1.15-1.3 (m, 2H), 1.4-1.55 (m, 1H), 1.65-1.8 (m, 4H), 1.95 (t, 2H), 2.4 (s, 3H), 2.42 (t, 2H), 2.85 (d, 2H), 3.25 (s, 3H), 3.42 (t, 2H), 4.0 (s, 3H), 4.22 (t, 2H), 6.15 (s, 1H), 6.85 (dd, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.38 (s, 1H), 7.59 (s, 1H), 8.5 (s, 1H). MS-ESI: 491 $[\text{MH}]^+$

元素分析	実測値	C	65.3	H	7.1	N	10.9
$\text{C}_{28}\text{H}_{34}\text{N}_4\text{O}_4 \cdot 1.3 \text{H}_2\text{O}$	理論値	C	65.4	H	7.2	N	10.9%

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^1H NMR スペクトル: (DMSO-d_6) 1.95-2.1 (m, 2H), 2.4 (br s, 4H), 2.45 (s, 3H), 2.5 (t, 2H), 3.65 (t, 4H), 3.75 (s, 3H), 4.0 (s, 3H), 4.25 (t, 2H), 6.25 (s, 1H), 6.95 (dd, 1H), 7.3 (s, 1H), 7.38 (s, 1H), 7.45 (d, 1H), 7.6 (s, 1H), 8.5 (s, 1H)

MS-ESI: 463 $[\text{MH}]^+$

元素分析	実測値	C	67.2	H	6.5	N	12.1
$\text{C}_{26}\text{H}_{30}\text{N}_4\text{O}_4$	理論値	C	67.5	H	6.5	N	12.1%

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^1H NMR スペクトル: (DMSO-d_6) 1.4 (s, 9H), 2.4 (s, 3H), 2.90 (s, 3H), 3.65 (t, 2H), 4.0 (s, 3H), 4.35 (t, 2H), 6.15 (s, 1H), 6.8 (dd, 1H), 7.28 (s, 1H), 7.35 (d, 1H), 7.42 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H);

MS-ESI: 479 $[\text{MH}]^+$

元素分析	実測値	C	65.0	H	6.4	N	11.7
$\text{C}_{26}\text{H}_{30}\text{N}_4\text{O}_5\text{S}$	理論値	C	65.3	H	6.3	N	11.7%

^1H NMR スペクトル: (DMSO-d_6) 2.4 (s, 3H), 2.5 (s, 3H), 2.9 (t, 2H), 4.0 (s, 3H), 4.25 (t, 2H), 6.25 (s, 1H), 6.9 (dd, 1H), 7.25 (s, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 8.5 (s, 1H), 11.0 (s, 1H)

MS-ESI: 379 $[\text{MH}]^+$

元素分析	実測値	C	64.6	H	5.8	N	14.2
$\text{C}_{21}\text{H}_{22}\text{N}_4\text{O}_3 \cdot 0.7 \text{H}_2\text{O}$	理論値	C	64.5	H	6.0	N	14.3%

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^1H NMR λ^{c} λ^{b} : (DMSO-d_6 , CF_3COOD) 1.6-1.8 (m, 2H), 2.05-2.2 (d, 2H),
2.2-2.3 (m, 1H), 2.45 (s, 3H), 3.2 (t, 2H), 3.65 (d, 2H), 4.1 (s, 3H), 4.22 (d, 2H),
4.6 (s, 2H), 6.2 (s, 0.5H, partially exchanged), 6.9 (dd, 1H), 7.35 (s, 1H), 7.4 (d,
1H), 7.55 (s, 1H), 7.8 (s, 1H), 9.1 (s, 1H)

MS-ESI: 458 $[\text{MH}]^+$

元素分析	実測値	C	67.6	H	6.1	N	15.2
$\text{C}_{26}\text{H}_{27}\text{N}_5\text{O}_3 \cdot 0.2 \text{H}_2\text{O}$	理論値	C	67.7	H	6.0	N	15.2%

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^1H NMR スペクトル: (DMSO-d_6) 2.07 (m, 2H), 2.78 (s, 3H), 2.87 (s, 3H), 3.25 (t, 2H), 3.97 (s, 3H), 4.23 (t, 2H), 6.43 (br s, 1H), 6.96 (dd, 1H), 7.32 (s, 1H), 7.41 (m, 3H), 7.59 (d, 1H), 8.48 (s, 1H) および 11.17 (s, 1H)

MS (ESI): 457 (MH)⁺

元素分析	実測値	C	57.5	H	5.3	N	12.0
$\text{C}_{22}\text{H}_{24}\text{N}_4\text{O}_5\text{S}$	理論値	C	57.9	H	5.3	N	12.3%

^1H NMR スペクトル: (DMSO-d_6) 1.37 (s, 9H), 1.94 (t, 2H), 3.13 (q, 2H), 3.97 (s, 3H), 4.21 (t, 2H), 6.89 (br s, 1H), 7.38 (s, 1H), 7.43 - 7.53 (m, 2H), 7.57 (s, 1H), 7.78 (dd, 1H) および 8.55 (s, 1H)

MS (ESI): 522 (MH)⁺

元素分析	実測値	C	52.1	H	4.7	N	7.9
$\text{C}_{22}\text{H}_{25}\text{N}_3\text{BrFO}_5$	理論値	C	52.3	H	4.9	N	8.0%

^1H NMR スペクトル: (DMSO-d_6) 1.87 (m, 2H), 2.73 (t, 2H), 3.98 (s, 3H), 4.26 (t, 2H), 7.40 (s, 1H), 7.50 (m, 2H), 7.55 (s, 1H), 7.78 (dd, 1H) および 8.55 (s, 1H)

MS (ESI): 422 (MH)⁺

¹H NMR (CDCl₃): 2.01 (m, 2H), 2.90 (s, 3H), 3.15 (t, 2H), 3.96 (s, 3H), 4.25 (t, 2H), 7.06 (s, 1H), 7.40 (s, 1H), 7.49 (m, 2H), 7.56 (s, 1H), 7.78 (dd, 1H) および 8.54 (s, 1H)
MS (ESI): 500/502 (MH)⁺

[illegible]

^1H NMR λ° C_6D_6 : (DMSO- d_6) 2.06 (m, 2H), 2.78 (s, 3H), 2.87 (s, 3H), 3.24 (t, 2H), 3.97 (s, 3H), 4.23 (t, 2H), 7.39 (s, 1H), 7.48 (m, 2H), 7.55 (s, 1H), 7.78 (dd, 1H) および 8.54 (s, 1H)
MS (ESI) : 514/516 (MH)⁺

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^1H NMR λ° C_6D_6 : (DMSO- d_6) 2.02 (m, 2H), 2.77 (s, 3H), 2.86 (s, 3H), 3.22 (t, 2H), 3.86 (s, 3H), 4.13 (t, 2H), 7.09 (s, 1H), 7.42 (s, 1H), 7.95 (s, 1H) および 12.02 (s, 1H)
MS (ESI) : 342 (MH)⁺

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^1H NMR スペクトル: (DMSO- d_6) 2.08 (m, 2H), 2.78 (s, 3H), 2.88 (s, 3H), 3.24 (t, 2H), 3.98 (s, 3H), 4.26 (t, 2H), 7.37 (s, 1H), 7.42 (s, 1H) および 8.86 (s, 1H)
MS (ESI): 360(MH)⁺

^1H NMR スペクトル: (DMSO- d_6) 2.06 (m, 2H), 2.38 (s, 3H), 2.79 (s, 3H), 2.89 (s, 3H), 3.24 (t, 2H), 3.96 (s, 3H), 4.21 (t, 2H), 6.11 (br s, 1H), 6.87 (dd, 1H), 7.23 (d, 1H), 7.30 (d, 1H), 7.35 (s, 1H), 7.57 (s, 1H), 8.46 (s, 1H) および 10.98 (s, 1H)

MS (ESI): 471 (MH)⁺

元素分析	実測値	C	58.3	H	5.6	N	11.7
$\text{C}_{23}\text{H}_{26}\text{N}_4\text{O}_5\text{S}$	理論値	C	58.7	H	5.6	N	11.9%

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^1H NMR スペクトル: (DMSO-d_6) 2.09 (m, 2H), 2.79 (s, 3H), 2.90 (s, 3H), 3.26 (t, 2H), 3.99 (s, 3H), 4.26 (t, 2H), 7.39 (s, 1H), 7.54 (dd, 1H), 7.56 (dd, 1H), 7.60 (s, 1H), 7.91 (d, 1H), 8.09 (d, 1H), 8.44 (d, 1H), 8.55 (s, 1H)および8.93 (dd, 1H)

MS (ESI) : 469 (MH)⁺

元素分析

実測値

C 58.6

H 5.1

N 11.9

$\text{C}_{23}\text{H}_{24}\text{N}_4\text{O}_5\text{S}$

理論値

C 59.0

H 5.2

N 12.0%

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¹H NMR (λ¹クトル: (DMSO-d₆) 2.09 (m, 2H), 2.71 (s, 3H), 2.79 (s, 3H), 2.89 (s, 3H), 3.25 (t, 2H), 3.98 (s, 3H), 4.25 (t, 2H), 7.37 (s, 1H), 7.38 (d, 1H), 7.61 (d, 1H), 7.63 (s, 1H), 7.89 (d, 1H), 8.20 (d, 1H), 8.54 (s, 1H)および 8.76 (d, 1H)
MS (ESI): 483 (MH)⁺
元素分析
実測値 C 59.1 H 5.3 N 11.5
理論値 C 59.1 H 5.0 N 12.0%

[illegible]

^1H NMR λ° クトル: (DMSO-d₆, 100°C) 1.24 (m, 1H), 1.59 (m, 1H), 1.70 (m, 1H), 1.83 (m, 1H), 2.05 (m, 2H), 2.17 (m, 1H), 2.24 (s, 3H), 2.64 (dt, 1H), 2.84 (dd, 1H), 4.05 (s, 3H), 4.18 (d, 2H), 7.43 (s, 1H), 7.69 (s, 1H), 7.87 (dd, 1H), 7.96 (d, 1H), 8.18 (s, 1H), 8.25 (dd, 1H), 8.59 (s, 1H)および9.16 (d, 1H)

MS (ESI): 499 (MH)⁺

元素分析	実測値	C	62.2	H	5.1	N	11.0
$\text{C}_{26}\text{H}_{25}\text{N}_4\text{F}_3\text{O}_3$	理論値	C	62.6	H	5.1	N	11.2%

^1H NMR λ° f f : (DMSO-d_6) 1.11 (m, 1H), 1.50 (m, 1H), 1.64 (m, 1H), 1.84 (m, 3H), 2.10 (m, 1H), 2.15 (s, 3H), 2.62 (d, 1H), 2.83 (d, 1H), 4.00 (s, 3H), 4.08 (d, 2H), 7.38 (s, 1H), 7.62 (s, 1H), 7.68 (dd, 1H), 7.97 (d, 1H), 8.10 (d, 1H), 8.34 (dd, 1H), 8.54 (s, 1H) および 8.97 (d, 1H)

MS (ESI): 449 (MH) $^+$

元素分析	実測値	C	66.2	H	5.6	N	12.3
$\text{C}_{25}\text{H}_{25}\text{N}_4\text{FO}_3 \cdot 0.2 \text{H}_2\text{O}$	理論値	C	66.4	H	5.7	N	12.4%

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^1H NMR λ° f f : (CDCl_3) 3.95 (s, 3H), 7.25 (dd, 1H), 7.37 (d, 1H), 7.67 (d, 1H) および 7.78 (d, 1H)

MS (ESI): 212 (MH) $^+$

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MS (ESI) : 178 (MH)⁺

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^1H NMR スペクトル: (DMSO-d_6) 1.11 (m, 1H), 1.68 (m, 5H), 2.10 (m, 1H), 2.20 (s, 3H), 2.64 (m, 4H), 2.87 (d, 1H), 3.98 (s, 3H), 4.09 (d, 2H), 7.37 (s, 1H), 7.57 (dd, 1H), 7.60 (s, 1H), 7.86 (d, 1H), 8.02 (d, 1H), 8.20 (d, 1H) および 8.53 (s, 1H)

MS (ESI): 463 (MH)⁺

元素分析	実測値	C	66.4	H	6.1	N	11.8
$\text{C}_{26}\text{H}_{27}\text{N}_4\text{FO}_3 \cdot 0.4 \text{H}_2\text{O}$	理論値	C	66.5	H	6.0	N	11.9%

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^1H NMR スペクトル: (CDCl_3) 2.70 (d, 3H), 3.94 (s, 3H), 7.17 (dd, 1H), 7.37 (d, 1H) および 7.61 (m, 2H)

MS (ESI): 192 (MH)⁺

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¹H NMR スペクトル: (DMSO-d₆) 1.37 (m, 2H), 1.51 (m, 4H), 1.95 (m, 2H), 2.32 (m, 4H), 2.42 (t, 2H), 3.98 (s, 3H), 4.23 (t, 2H), 7.38 (s, 1H), 7.56 (m, 2H), 7.62 (s, 1H), 7.91 (d, 1H), 8.09 (d, 1H), 8.44 (d, 1H), 8.54 (s, 1H)および8.91 (dd, 1H)

MS (ESI) : 445 (MH)⁺

元素分析	実測値	C 70.9	H 6.3	N 12.7
$C_{26}H_{28}N_4O_3$	理論値	C 70.3	H 6.3	N 12.6%

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^1H NMR スペクトル: (DMSO- d_6) 2.07 (m, 2H), 2.12 (s, 3H), 2.31 (s, 3H), 2.79 (s, 3H), 2.89 (s, 3H), 3.25 (t, 2H), 3.97 (s, 3H), 4.23 (t, 2H), 6.86 (dd, 1H), 7.20 (d, 1H), 7.25 (d, 1H), 7.35 (s, 1H), 7.58 (s, 1H), 8.46 (s, 1H)および 11.17 (s, 1H)

MS (ESI) : 485 (MH) $^+$

元素分析	実測値	C	59.5	H	5.8	N	11.4
$\text{C}_{24}\text{H}_{28}\text{N}_4\text{O}_5\text{S}$	理論値	C	59.5	H	5.8	N	11.6%

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^1H NMR スペクトル: (DMSO-d_6) 2.38 (s, 3H), 2.45 (m, 6H), 3.57 (t, 4H), 3.95 (s, 3H), 4.03 - 4.14 (m, 2H), 4.23 (m, 1H), 4.95 (s, 1H), 6.12 (s, 1H), 6.86 (dd, 1H), 7.23 (d, 1H), 7.29 (d, 1H), 7.37 (s, 1H), 7.57 (s, 1H), 8.47 (s, 1H)および 10.98 (s, 1H)

MS (ESI): 465 (MH)⁺

元素分析	実測値	C	62.7	H	5.9	N	11.5
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_5 \cdot 0.7\text{H}_2\text{O}$	理論値	C	62.9	H	6.2	N	11.7%

^1H NMR スペクトル: (DMSO-d_6) 1.35 (m, 2H), 1.51 (m, 4H), 2.39 (m, 9H), 3.96 (s, 3H), 4.08 (m, 2H), 4.21 (dd, 1H), 4.86 (br s, 1H), 6.11 (s, 1H), 6.87 (dd, 1H), 7.23 (d, 1H), 7.29 (d, 1H), 7.37 (s, 1H), 7.56 (s, 1H), 8.45 (s, 1H)および 10.98 (s, 1H)

MS (ESI): 464 (MH)⁺

元素分析	実測値	C	66.2	H	6.4	N	11.9
$\text{C}_{26}\text{H}_{30}\text{N}_4\text{O}_4 \cdot 0.4\text{H}_2\text{O}$	理論値	C	66.5	H	6.6	N	11.9%

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^1H NMR スペクトル: (DMSO-d_6) 2.38 (s, 3H), 2.76 (m, 1H), 2.90 (t, 1H), 3.43 (m, 1H), 3.97 (s, 3H), 4.04 (m, 1H), 4.57 (dd, 1H), 6.11 (s, 1H), 6.86 (dd, 1H), 7.27 (m, 2H), 7.38 (s, 1H), 7.59 (s, 1H), 8.46 (s, 1H)および 10.92 (s, 1H)

MS (ESI): 378 (MH)⁺

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¹H NMR (λ^νクロム): (DMSO-d₆) 1.69 (br s, 4H), 2.38 (s, 3H), 2.50 (m, 6H), 3.97 (s, 3H), 4.07 (m, 2H), 4.21 (dd, 1H), 4.96 (br s, 1H), 6.11 (s, 1H), 6.86 (dd, 1H), 7.23 (d, 1H), 7.29 (d, 1H), 7.35 (s, 1H), 7.56 (s, 1H), 8.46 (s, 1H)および10.98 (s, 1H)
MS (ESI): 450 (MH)⁺
元素分析
実測値 C 65.5 H 6.3 N 11.8
理論値 C 65.9 H 6.4 N 12.3%
C₂₅H₂₈N₄O₄・0.4H₂O

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^1H NMR スペクトル: (DMSO-d_6) 0.96 (t, 6H), 2.38 (s, 3H), 2.52 (m, 6H), 3.96 (s, 3H), 3.97 (m, 1H), 4.09 (m, 1H), 4.23 (dd, 1H), 4.84 (br s, 1H), 6.12 (s, 1H), 6.88 (dd, 1H), 7.24 (d, 1H), 7.29 (d, 1H), 7.36 (s, 1H), 7.56 (s, 1H), 8.45 (s, 1H) および 10.98 (s, 1H)

MS (ESI): 452 (MH)⁺

元素分析	実測値	C	66.2	H	6.7	N	12.4
$\text{C}_{25}\text{H}_{30}\text{N}_4\text{O}_4$	理論値	C	66.6	H	6.7	N	12.4%

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^1H NMR スペクトル: (DMSO-d_6) : 2.11 (s, 3H), 2.29 (m, 4H), 2.40 (s, 3H), 2.47 (m, 6H), 3.96 (s, 3H), 4.07 (m, 2H), 4.20 (dd, 1H), 4.89 (d, 1H), 6.11 (s, 1H), 6.87 (dd, 1H), 7.23 (d, 1H), 7.29 (d, 1H), 7.35 (s, 1H), 7.58 (s, 1H), 8.46 (s, 1H) および 10.98 (s, 1H)

MS (ESI): 479 (MH)⁺

元素分析	実測値	C	64.4	H	6.5	N	14.4
$\text{C}_{26}\text{H}_{31}\text{N}_5\text{O}_4 \cdot 0.3\text{H}_2\text{O}$	理論値	C	64.7	H	6.6	N	14.5%

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¹H NMR スペクトル: (DMSO-d₆) 1.00 (d, 6H), 2.40 (s, 3H), 2.56 - 2.78 (m, 3H), 3.97 (m, 4H), 4.07 - 4.28 (m, 2H), 5.04 (m, 1H), 6.12 (s, 1H), 6.88 (dd, 1H), 7.22 - 7.33 (m, 2H), 7.38 (s, 1H), 7.58 (s, 1H), 8.48 (s, 1H)および10.98 (s, 1H)

MS (ESI) : 437 (MH)⁺

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MS (ESI) : 501 (MH)⁺

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¹H NMR (A₂ 70%): (CDCl₃) 4.48 (s, 1H), 6.48 (m, 1H), 7.14 (s, 1H), 7.32 (t, 1H), 7.57 (s, 1H)および8.20 (br s, 1H)
MS (ESI): 200 (M-H)⁺

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¹H NMR スペクトル: (DMSO-d₆) 1.38 (m, 2H), 1.47 (m, 4H), 1.95 (m, 2H), 2.32 (m, 4H), 2.40 (m, 2H), 3.66 (3H, s), 3.97 (s, 3H), 4.28 (t, 2H), 6.35 (br s, 1H), 7.06 (s, 1H), 7.24 (t, 1H), 7.34 (s, 1H), 7.36 (s, 1H), 7.55 (s, 1H) および 8.41 (s, 1H)

MS (ESI) : 463 (MH)⁺

元素分析

実測値 C 65.2 H 6.8 N 11.2

$$\text{C}_{26}\text{H}_{30}\text{N}_4\text{O}_4 \cdot 1.0 \text{H}_2\text{O}, 0.3 \text{ ジ・エチルエーテル}$$

理論値 C 64.9 H 7.0 N 11.1%

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^1H NMR スペクトル: (CDCl_3) 3.92 (s, 3H), 5.40 (s, 1H), 6.42 (br s, 1H), 6.87 (s, 1H), 7.07 (m, 1H), 7.13 (s, 1H), 7.93 (br s, 1H)

MS (ESI): 162 (M-H)⁺

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^1H NMR スペクトル: (DMSO-d_6) 1.39 (m, 2H), 1.50 (m, 4H), 1.98 (t, 2H), 2.35 (m, 4H), 2.40 (t, 2H), 3.98 (s, 3H), 4.25 (t, 2H), 6.10 (t, 1H), 6.90 (d, 1H), 7.15 (t, 1H), 7.30 (t, 1H), 7.35 (d, 1H), 7.38 (s, 1H), 7.62 (s, 1H), 8.45 (s, 1H) および 11.29 (s, 1H)

MS (ESI): 433 (MH)⁺

m.p. 80 - 82 °C

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¹H NMR スペクトル: (DMSO-d₆) 1.39 (m, 2H), 1.50 (m, 4H), 2.35 (m, 4H), 2.40 (t, 2H), 3.98 (s, 3H), 4.25 (t, 2H), 7.05 (dd, 1H), 7.15 (t, 1H), 7.35 (t, 1H), 7.38 (s, 1H), 7.40 (s, 1H), 7.50 (d, 1H), 7.60 (s, 1H), 8.10 (d, 1H), 8.15 (d, 1H), 8.55 (s, 1H) および 11.33 (s, 1H)

MS (ESI) : 483 (MH)⁺

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^1H NMR スペクトル: (DMSO-d_6) 1.30 (t, 3H), 1.40 (m, 2H), 1.50 (m, 4H), 1.98 (t, 2H), 2.35 (m, 4H), 2.40 (t, 2H), 3.98 (s, 3H), 4.25 (t, 2H), 4.30 (q, 2H), 7.15 (m, 1H), 7.18 (s, 1H), 7.60 (s, 1H), 8.40 (s, 1H) および δ 12.60 (s, 1H)

MS (ESI) : 539 (MH) $^+$

元素分析	実測値	C	61.2	H	5.9	N	10.3
$\text{C}_{28}\text{H}_{31}\text{ClN}_4\text{O}_5 \cdot 0.5 \text{H}_2\text{O}$	理論値	C	61.4	H	5.9	N	10.2%

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^1H NMR スペクトル: (CDCl_3) 1.40 (t, 3H), 3.98 (s, 3H), 4.40 (q, 2H), 6.60 (d, 1H),
7.05 (d, 1H), 7.15 (s, 1H)および9.10 (s, 1H)
MS (ESI): 254 (MH)⁺

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^1H NMR スペクトル: (DMSO-d_6) 1.38 (t, 3H), 4.35 (q, 2H), 6.60 (d, 1H), 6.95 (d,
1H), 7.10 (d, 1H), 9.80 (s, 1H)および11.80 (s, 1H)
MS (ESI): 238 (MH)⁺

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^1H NMR スペクトル: (CDCl_3) 2.10 (s, 3H), 2.30 (s, 3H), 3.98 (s, 3H), 5.30 (s, 2H),
6.85 (dd, 1H), 7.20 (d, 1H), 7.25 (d, 1H), 7.40 (m, 6H), 7.60 (s, 1H), 8.40 (s,
1H)および 10.74 (s, 1H)

MS (ESI) : 426 (MH) $^+$

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^1H NMR スペクトル: (CDCl_3) 1.70 (s, 9H), 2.08 (s, 3H), 2.50 (s, 3H), 4.10 (s, 3H),
5.35 (s, 2H), 7.15 (dd, 1H), 7.38 (m, 6H), 7.60 (s, 1H), 8.20 (d, 1H)および 8.60
(s, 1H)

MS (ESI) : 526 (MH) $^+$

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MS (ESI) : 447 (MH)⁺

元素分析	実測値	C 66.8	H 5.9	N 12.4
$C_{25}H_{26}N_4O_4 \cdot 0.2 H_2O$	理論値	C 66.7	H 5.9	N 12.4%

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MS (ESI) : 447 (MH)⁺

$$\text{C}_{25}\text{H}_{26}\text{N}_4\text{O}_4 \cdot 0.4 \text{H}_2\text{O} \quad \text{理論值} \quad \text{C} \ 66.2 \quad \text{H} \ 6.0 \quad \text{N} \ 12.4\%$$

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MS (ESI) : 460 (MH)⁺

$C_{26}H_{28}N_4O_3 \cdot 0.3 H_2O$	理論值	C	67.2	H	6.4	N	15.1%
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m.p. 179-180°C

^1H NMR λ^\vee C_6H_5 : (DMSO- d_6) 3.99(s, 3H); 5.36(s, 2H); 7.35-7.5(m, 4H); 7.55-7.65(m, 5H); 7.72(d, 1H); 8.6(s, 1H)

MS - ESI: 411 [MH] $^+$

元素分析 :

実測値 C 63.38 H 4.07 N 6.78

$\text{C}_{22}\text{H}_{16}\text{ClFN}_2\text{O}_3 \cdot 0.06\text{H}_2\text{O} \cdot 0.05\text{CH}_2\text{Cl}_2$

理論値 C 63.64 H 3.93 N 6.73%

^1H NMR λ^\vee C_6H_5 : (DMSO- d_6) 4.0(s, 3H); 7.27(s, 1H); 7.43(dd, 1H); 7.56(t, 1H); 7.57(s, 1H); 7.72(dd, 1H); 8.5(s, 1H)

MS - ESI: 321 [MH] $^+$

[illegible]

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[illegible]

元素分析	実測値	C	59.6	H	5.7	N	12.2
$C_{23}H_{26}ClFN_4O_3$	理論値	C	59.9	H	5.7	N	12.2%

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^1H NMR スペクトル: (DMSO-d_6) 3.25 (s, 3H), 3.50 (t, 2H), 3.60 (t, 2H), 3.80 (t, 2H), 4.00 (s, 3H), 4.30 (t, 2H), 7.40 (s, 1H), 7.55 (m, 1H), 7.60 (m, 1H), 7.65 (s, 1H), 7.90 (d, 1H), 8.10 (d, 1H), 8.40 (m, 1H), 8.50 (s, 1H) および 8.90 (m, 1H)

MS (ESI): 422 (MH^+)

元素分析	実測値	C	65.8	H	5.2	N	10.0
$\text{C}_{22}\text{H}_{23}\text{N}_3\text{O}_5$	理論値	C	65.6	H	5.5	N	10.0%

^1H NMR スペクトル: (DMSO-d_6) 1.13(s, 9 H); 3.26(s, 3H); 3.5(m, 2H); 3.65(m, 2H); 3.85(m, 2H); 3.91(s, 3H); 4.3(m, 2H); 5.9(s, 2H); 7.2(s, 1H); 7.5(s, 1H); 8.4(s, 1H)

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¹H NMR (DMSO-d₆): (3.25(s, 3H); 3.45(t, 2H); 3.6(t, 2H); 3.8(t, 2H); 3.9(s, 3H); 4.2(t, 2H); 7.15(s, 1H); 7.45(s, 1H); 8.0(s, 1H)
MS - EI: 294 [M]⁺

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¹H NMR (DMSO-d₆) 3.24(s, 3H); 3.47(m, 2H); 3.62(m, 2H); 3.84(t, 2H); 4.01(s, 3H); 4.25(t, 2H); 7.41(s, 1H); 7.49(s, 1H); 8.88(s, 1H)

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^1H NMR スペクトル: (DMSO- d_6) 1.37 (m, 2H), 1.50 (m, 4H), 1.95 (m, 2H), 2.21 (s, 3H), 2.34 (m, 4H), 2.42 (t, 2H), 3.96 (s, 3H), 4.22 (t, 2H), 6.95 (dd, 1H), 7.16 (s, 1H), 7.35 (m, 3H), 7.58 (s, 1H), 8.48 (s, 1H)および 10.82 (s, 1H)

MS (ESI) : 447 (MH) $^+$

元素分析	実測値	C	68.2	H	6.8	N	12.6
$\text{C}_{26}\text{H}_{30}\text{N}_4\text{O}_3 \cdot 0.5 \text{H}_2\text{O}$,	理論値	C	68.5	H	6.8	N	12.3%

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^1H NMR スペクトル: (DMSO-d_6) 1.68 (m, 4H), 1.97 (m, 2H), 2.22 (s, 3H), 2.43 (m, 4H), 2.55 (t, 2H), 3.96 (s, 3H), 4.22 (t, 2H), 6.93 (dd, 1H), 7.16 (s, 1H), 7.35 (m, 3H), 7.58 (s, 1H), 8.48 (s, 1H)および 10.82 (br s, 1H)

MS (ESI): 433 (MH)⁺

m.p. 75-77°C

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^1H NMR スペクトル: (DMSO-d_6) 1.38 (m, 2H), 1.50 (m, 4H), 2.24 (s, 3H), 2.73 (t, 2H), 3.96 (s, 3H), 4.28 (t, 2H), 6.93 (dd, 1H), 7.16 (s, 1H), 7.32 (d, 1H), 7.37 (m, 2H), 7.58 (s, 1H), 8.47 (s, 1H)および 10.82 (br s, 1H)

MS (ESI): 433 (MH)⁺

元素分析	実測値	C	67.0	H	6.5	N	13.0
$\text{C}_{25}\text{H}_{23}\text{N}_4\text{O}_3 \cdot 0.75 \text{H}_2\text{O}$	理論値	C	67.3	H	6.6	N	12.6%

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^1H NMR スペクトル: ($\text{DMSO}-d_6$) 1.38(m, 2H); 1.50(m, 4H); 2.4-2.5(m, 4H);
2.75(t, 2H); 3.95(s, 3H); 4.27(t, 2H); 7.30(m, 3H); 7.40(s, 1H); 7.46(m, 2H);
7.54(s, 1H); 8.52(s, 1H)
MS - ESI: 380 $[\text{MH}]^+$

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MS (ESI) : 471 (MH)⁺

元素分析	実測値	C 57.0	H 5.6	N 11.4
$C_{23}H_{26}F_4N_4O_5S \cdot 0.5 H_2O$	理論値	C 57.5	H 5.7	N 11.7%

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m.p. 184.0 - 185.5°C

^1H NMR λ° DMSO-d_6 : 1.70 (m, 4H), 1.99 (m, 2H), 2.46 (m, 4H), 2.58 (t, 2H), 4.00 (s, 3H), 4.26 (t, 2H), 6.48 (t, 1H), 7.36 (s, 1H), 7.55 (t, 1H), 7.60 (s, 1H), 7.92 (d, 1H), 8.19 (d, 1H), 8.50 (s, 1H) および 11.78 (br s, 1H)

MS (ESI): 420 (MH) $^+$

元素分析	実測値	C	63.9	H	5.9	N	16.1
$\text{C}_{23}\text{H}_{23}\text{N}_5\text{O}_3 \cdot 0.7 \text{H}_2\text{O}$	理論値	C	63.9	H	6.2	N	16.2%

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m.p. 206-209°C

^1H NMR λ° クトル: (DMSO- d_6) 6.25 (s, 1H), 7.27 (s, 1H), 7.33 (s, 1H), 7.82 (s, 1H), 9.00 (s, 1H) および 11.20 (s, 1H)

MS (ESI): 135 (MH) $^+$

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^1H NMR λ° クトル: (DMSO- d_6) 1.43 (m, 2H), 1.56 (m, 4H), 2.04 (m, 2H), 2.59 (m, 6H), 3.97 (s, 3H), 4.24 (t, 2H), 7.01 (s, 1H), 7.11 (dd, 1H), 7.36 (s, 1H), 7.48 (m, 2H), 7.58 (s, 1H), 8.48 (s, 1H) および 11.53 (br s, 1H)

MS (ESI): 477 (MH) $^+$

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^1H NMR λ° 713: (DMSO- d_6) 2.26 (m, 2H); 3.08 (s, 3H); 3.35 (m, 2H); 4.03 (s, 3H); 4.38 (m, 2H); 7.45 (s, 1H); 7.60 (m, 1H); 7.65 (m, 1H); 7.70 (s, 1H); 7.95 (d, 1H); 8.15 (d, 1H); 8.46 (d, 1H); 8.60 (s, 1H); 8.95 (d, 1H)

MS (ESI): 440 [MH] $^{+}$

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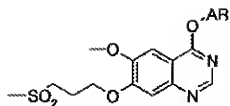
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表 X



実施例 番号	重量 (mg)	収量 %	MS-ESI [MH] ⁺	AR	註
185	199	93	474		a
186	171	85	422		b
187	183	88	460		c
188	83	40	455		d

¹H NMR スペクトル: (DMSO-d₆) 2.24 (m, 2H); 3.04 (s, 3H); 3.35 (m, 2H); 3.99 (s, 3H); 4.32 (m, 2H); 7.42 (s, 1H); 7.64 (s, 1H); 7.80 (d, 2H); 8.04 (d, 1H); 8.29 (d, 1H); 8.55 (s, 1H); 8.87 (d, 1H)

^1H NMR λ° H_2O : (DMSO- d_6) 2.24 (m, 2H); 2.40 (s, 3H); 3.05 (s, 3H); 3.35 (m, 2H); 4.0 (s, 3H); 4.32 (m, 2H); 6.13 (s, 1H); 6.88 (d, 1H); 7.25 (d, 1H); 7.32 (d, 1H); 7.39 (s, 1H); 7.60 (s, 1H); 8.50 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 2.24 (m, 2H); 2.28 (s, 3H); 3.05 (s, 3H); 3.35 (m, 2H); 4.0 (s, 3H); 4.32 (m, 2H); 7.36 (d, 1H); 7.41 (s, 1H); 7.65 (s, 1H); 7.87 (d, 1H); 8.11 (d, 1H); 8.53 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 2.24 (m, 2H); 3.05 (s, 3H); 3.35 (m, 2H); 3.98 (s, 3H); 4.32 (m, 2H); 7.06 (d, 1H); 7.12 (s, 1H); 7.18 (d, 1H); 7.40 (d, 1H); 7.59 (m, 2H); 7.85 (m, 2H); 8.55 (d, 1H); 9.8 (br s, 1H)

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¹H NMR スペクトル: (DMSO-d₆ + TFA) 1.60 (m, 2H); 2.05 (d, 2H); 2.15 (m, 1H); 2.80 (s, 3H); 3.05 (m, 2H); 3.55 (m, 2H); 4.05 (s, 3H); 4.15 (d, 2H); 7.20 (dd, 1H); 7.50 (dd, 2H); 7.65 (d, 1H); 7.70 (s, 1H); 8.80 (s, 1H)
MS (ESI): 454 [MH]⁺

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MS (ESI) : 434 [MH]⁺

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^1H NMR λ° C_6H_5 ($\text{DMSO-d}_6 + \text{TFA}$) 2.75 (s, 3H); 3.85 (s, 3H); 7.15 (dd, 1H);
7.25 (s, 1H); 7.70 (d, 1H)

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^1H NMR λ° C_6H_5 (DMSO-d_6) 2.70 (s, 3H); 6.95 (dd, 1H); 7.00 (d, 1H); 7.55 (d,
1H)

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^1H NMR λ° H : (DMSO-d_6 + TFA) 1.60 (m, 2H); 2.10 (m, 3H); 2.85 (s, 3H);
3.05 (m, 2H); 3.55 (m, 2H); 4.05 (s, 3H); 4.20 (d, 2H); 7.55 (s, 1H); 7.80 (s,
1H); 7.85 (dd, 1H); 8.15 (s, 1H); 8.3 (d, 1H); 8.85 (s, 1H); 9.20 (s, 1H); 9.25 (s,
1H)

MS (ESI) : 456 $[\text{MH}]^+$ 456

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^1H NMR λ° H : (DMSO-d_6) 1.25 (t, 3H); 3.85 (s, 3H); 4.20 (q, 2H); 6.95 (d,
1H); 7.00 (s, 1H); 8.05 (d, 1H); 8.50 (s, 1H)

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^1H NMR λ° DMSO-d_6 : 1.40 (t, 3H); 4.00 (s, 3H); 4.45 (q, 2H); 7.45 (dd, 1H); 7.55 (d, 1H); 8.30 (d, 1H); 9.10 (s, 1H)

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^1H NMR λ° DMSO-d_6 : 1.40 (t, 3H); 3.95 (s, 3H); 4.40 (q, 2H); 7.35 (dd, 1H); 7.50 (d, 1H); 8.15 (d, 1H); 8.90 (d, 1H); 9.25 (d, 1H)

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^1H NMR λ° DMSO-d_6 : 3.95 (s, 3H); 7.35 (dd, 1H); 7.45 (d, 1H); 7.60 (br s, 1H); 8.00 (d, 1H); 8.20 (br s, 1H); 8.75 (s, 1H); 9.25 (s, 1H)

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¹H NMR spectrum (DMSO-d₆) 4.00 (t, 3H); 7.40 (dd, 1H); 7.50 (d, 1H); 8.00 (d, 1H); 8.95 (s, 1H); 9.10 (d, 1H)

¹H NMR (DMSO-d₆) 7.25 (d, 1H); 7.30 (d, 1H); 7.95 (d, 1H); 8.85 (d, 1H); 9.00 (d, 1H)

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^1H NMR スペクトル: (CDCl_3) 1.95 (m, 2H); 2.15 (m, 2H); 2.45 (m, 4H); 2.60 (t, 2H); 2.80 (t, 2H); 3.35 (t, 2H); 3.75 (m, 4H); 3.90 (br s, 1H); 4.05 (s, 3H); 4.30 (t, 2H); 6.55 (d, 1H); 6.85 (m, 2H); 7.30 (s, 1H); 7.55 (s, 1H); 8.65 (s, 1H)

MS (ESI) : 451 $[\text{MH}]^+$

元素分析	:	実測値	C	66.4	H	6.9	N	12.4
$\text{C}_2\text{H}_4\text{N}_4\text{O}_4$; 1 HCl, 2 H_2O		理論値	C	66.7	H	6.7	N	12.4%

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^1H NMR スペクトル (DMSO-d_6) 1.75 (m, 2H); 2.60 (m, 2H); 3.05 (m, 2H); 4.90 (br s, 1H); 6.30 (m, 3H); 8.25 (br s, 1H)

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^1H NMR λ° δ (DMSO- d_6) 1.50 (m, 9H); 1.90 (m, 2H); 2.70 (t, 2H); 3.65 (t, 2H); 4.75 (br s, 1H); 6.55 (d, 1H); 6.65 (dd, 1H); 7.45 (d, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 1.55 (s, 9H); 1.95 (m, 2H); 2.15 (m, 2H); 2.50 (m, 4H); 2.60 (t, 2H); 2.85 (t, 2H); 3.75 (m, 6H); 4.05 (s, 3H); 4.30 (t, 2H); 7.00 (m, 2H); 7.35 (s, 1H); 7.55 (s, 1H); 7.80 (d, 1H); 8.65 (s, 1H)

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^1H NMR λ° H_2O : (CDCl_3) 1.90 (br, 4H); 2.30 (br, 2H); 2.70 (br d, 6H); 3.10 (t, 2H); 3.65 (t, 2H); 4.05 (s, 3H); 4.30 (t, 2H); 6.70 (d, 1H); 6.80 (dd, 1H); 7.00 (s, 1H); 7.30 (s, 1H); 7.55 (s, 1H); 8.65 (s, 1H)
MS (ESI): 421 $[\text{MH}]^+$

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^1H NMR スペクトル: (DMSO-d_6 , TFA) 3.15 (t, 2H); 3.70 (t, 2H); 6.75 (dd, 1H);
6.85 (d, 1H); 7.30 (d, 1H)

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^1H NMR スペクトル: (CDCl_3) 3.05 (t, 2H); 3.95 (br s, 2H); 4.70 (br s, 1H); 6.60
(d, 1H); 6.65 (s, 1H); 7.70 (br s, 1H)

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^1H NMR λ° DMSO-d_6 : 1.60 (s, 9H); 1.80 (m, 4H); 2.20 (m, 2H); 2.55 (m, 4H); 2.70 (t, 2H); 3.15 (t, 2H); 4.05 (br s, 5H); 4.30 (t, 2H); 7.00 (d, 1H); 7.05 (s, 1H); 7.30 (s, 1H); 7.55 (s, 1H); 7.90 (br s, 1H); 8.60 (s, 1H)

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^1H NMR λ° CDCl_3 : 1.65 (m, 2H); 2.00 (m, 3H); 2.25 (m, 2H); 2.45 (s, 3H); 3.10 (m, 4H); 3.65 (t, 2H); 4.05 (s, 3H); 4.10 (d, 2H); 6.70 (d, 1H); 6.85 (dd, 1H); 7.0 (s, 1H); 7.25 (s, 1H); 7.55 (s, 1H); 8.60 (s, 1H)

MS (ESI) : 421 $[\text{MH}]^+$

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^1H NMR λ° CDCl_3 : 1.50 (br s, 1H); 2.00 (m, 5H); 2.30 (s, 3H); 2.90 (d, 2H); 3.15 (t, 2H); 4.05 (br s, 7H); 7.05 (br s, 2H); 7.30 (s, 1H); 7.55 (s, 1H); 7.95 (br s, 1H); 8.60 (s, 1H)

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^1H NMR λ° CDCl_3 : d_H (300MHz, CDCl_3): 1.5 (2H, m; $\text{NCH}_2\text{CH}_2\text{CH}_2$), 1.6 (4H, m; 2 x NCH_2CH_2), 2.6 (4H, t; 2 x NCH_2), 2.9 (2H, t; NCH_2), 4.1 (3H, s; OCH_3), 4.3 (2H, t; OCH_2), 7.3 (1H, s; ArH), 7.4 (1H, dd; ArH), 7.5 (1H, dd; ArH), 7.6 (1H, s; ArH), 7.9 (1H, d; ArH), 8.0 (1H, d; ArH), 8.2 (1H, d; ArH), 8.6 (1H, s; ArH) および 8.9 (1H, dd; ArH)
 m/z (ESP+) 431 (MH^+ , 100%)

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^1H NMR スペクトル: d_{H} (300MHz, DMSO- d_6): 4.0 (3H, s; OCH_3), 5.4 (2H, s; OCH_2), 7.3-7.7 (9H, m; 9 x ArH), 7.9 (1H, br s; ArH), 8.1 (1H, d; ArH), 8.4 (1H, d; ArH), 8.5 (1H, s; ArH) および 8.9 (1H, d; ArH)

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^1H NMR スペクトル: d_{H} (300MHz, DMSO- d_6): 4.0 (3H, s; OCH_3), 7.1 (1H, s; ArH), 7.3-7.4 (3H, m; 3 x ArH), 7.9 (1H, br s; ArH), 8.1 (1H, d; ArH), 8.4-8.5 (2H, d; 2 x ArH) および 8.9 (1H, d; ArH)

m/z (ESP+) 320 (MH^+ , 100%)

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^1H NMR λ° δ (300MHz, CDCl_3): 2.7 (4H, t; 2 x NCH_2), 3.0 (2H, t; NCH_2), 3.7 (4H, t; 2 x OCH_2), 4.1 (3H, s; OCH_3), 4.4 (2H, t; OCH_2), 7.2 (1H, s; ArH), 7.4 (1H, dd; ArH), 7.5 (1H, dd; ArH), 7.6 (1H, s; ArH), 7.9 (1H, d; ArH), 8.0 (1H, br s; ArH), 8.2 (1H, d; ArH), 8.6 (1H, s; ArH) および 8.9 (1H, dd; ArH)

m/z (ESP+) 433 (MH^+ , 100%)

元素分析	実測値	C	65.0	H	5.6	N	12.6
$\text{C}_{24}\text{H}_{24}\text{N}_4\text{O}_4 \cdot 0.5\text{H}_2\text{O}$	理論値	C	65.3	H	5.7	N	12.7%

^1H NMR λ° δ (300MHz, CDCl_3): 2.3-2.5 (4H, m; 2 x pyrrolidinone- CH_2), 4.0-4.1 (4H, m; pyrrolidinone- CH ; OCH_3), 4.2-4.3 (2H, m; OCH_2), 6.1 (1H, br s; NH), 7.3 (1H, s; ArH), 7.4 (1H, dd; ArH), 7.5 (1H, dd; ArH), 7.9 (1H, d; ArH), 8.0 (1H, br s; ArH), 8.2 (1H, d; ArH), 8.6 (1H, s; ArH) および 8.9 (1H, dd; ArH)

m/z (ESP+) 417 (MH^+ , 100%)

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^1H NMR λ^{a} δ (ppm): d_{H} (300MHz, DMSO- d_6) 1.7 (4H, m; 2 x pyrrolidine- CH_2), 2.0 (2H, t; OCH_2CH_2), 2.5 (4H, m; 2 x pyrrolidine- NCH_2), 2.6 (2H, t; NCH_2), 4.0 (3H, s; OCH_3), 4.2 (2H, t; OCH_2), 7.1 (1H, br d; ArH), 7.2 (1H, t; ArH), 7.3-7.4 (3H, m; 3 x ArH), 7.5 (1H, br d; ArH), 7.6 (1H, s; ArH), 8.1-8.2 (2H, m; 2 x ArH), 8.5 (1H, s; ArH), 11.3 (1H, s; carbazole NH)
 m/z (ESP+) 469 (MH^+ , 100%)

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MS-ESI : 510-512 [MH]⁺

¹H NMR 測定条件: (DMSO-d₆) 3.12 (s, 3H) ; 3.85 (s, 3H) ; 4.1 (t, 2H) ; 4.45 (t, 2H) ; 6.45 (s, 1H) ; 7.2 (s, 1H) ; 7.3 (s, 1H) ; 7.35 (m, 2H) ; 7.42 (d, 1H) ; 7.8 (s, 1H) ; 7.85 (s, 1H) ; 8.35 (s, 1H) ; 9.45 (s, 1H)

¹H NMR 測定条件: (DMSO-d₆) 4.05 (s, 3H) ; 5.35 (s, 2H) ; 6.5 (s, 1H) ; 7.3 (d, 1H) ; 7.4-7.65 (m, 9H) ; 7.8 (s, 1H) ; 8.3 (s, 1H) ; 8.7 (s, 1H)

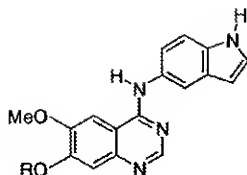
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MS-ESI : 307 [MH]⁺

¹H NMR λ[°] 71.7; (DMSO-d₆) 3.98 (s, 3H) ; 6.42 (s, 1H) ; 7.0 (s, 1H) ; 7.3-7.45
(m, 3H) ; 7.85 (s, 2H) ; 8.28 (s, 1H) ; 9.35 (s, 1H) ; 10.25 (br s, 1H) ; 11.05 (s,
1H)

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表 XI



実施例 番号	重量 (mg)	収量%	MS-ESI [MH] ⁺	註	R
202	83	59	441	a	
203	91	72	398	b	
204	76	55	432	c	

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¹H NMR スペクトル: (DMSO-d₆) 3.08 (s, 3H); 3.9 (t, 2H); 3.95 (s, 3H); 4.35 (t, 2H); 6.45 (s, 1H); 6.75 (d, 2H); 7.15 (s, 1H); 7.35 (m, 2H); 7.4 (d, 1H); 7.85 (s, 1H); 7.9 (s, 1H); 8.15 (d, 2H); 8.38 (s, 1H); 9.45 (s, 1H)

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^1H NMR λ^* C_6D_6 : (DMSO- d_6) 4.0 (s, 3H) ; 5.35 (s, 2H) ; 6.42 (s, 1H) ; 7.3-7.55 (m, 5H) ; 7.8-8.0 (m, 3H) ; 8.4 (s, 1H) ; 8.6 (d, 1H) ; 8.75 (s, 1H) ; 9.5 (s, 1H)

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^1H NMR λ^* C_6D_6 : (DMSO- d_6) 2.45 (s, 3H) ; 3.32 (t, 2H) ; 3.95 (s, 3H) ; 4.32 (t, 2H) ; 6.45 (s, 1H) ; 7.15 (s, 1H) ; 7.3-7.45 (m, 3H) ; 7.85 (s, 1H) ; 7.9 (s, 1H) ; 8.35 (s, 1H) ; 8.85 (s, 1H) ; 9.45 (s, 1H)

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MS-ESI : 448 [MH]⁺

¹H NMR λ[°] ʁɪʁ: (DMSO_d₆) 2.0 (m, 2H) ; 2.4 (s, 3H) ; 2.3-2.6 (m, 6H) ; 3.6 (t, 4H) ; 3.95 (s, 3H) ; 4.2 (t, 2H) ; 6.12 (s, 1H) ; 7.12 (s, 1H) ; 7.3 (br s, 2H) ; 7.7 (s, 1H) ; 7.85 (s, 1H) ; 8.35 (s, 1H) ; 9.4 (s, 1H)

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¹H NMR λ[°] ʁɪʁ: (DMSO_d₆) 2.3 (s, 3H) ; 4.3 (br s, 2H) ; 5.8 (s, 1H) ; 6.35 (d, 1H) ; 6.55 (s, 1H) ; 6.95 (d, 1H) ; 10.35 (br s, 1H)

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MS-ESI : 411 [MH]⁺

¹H NMR λ[°] ʁɪʁ: (DMSO_d₆) 2.41 (s, 3H) ; 4.01 (s, 3H) ; 5.33 (s, 2H) ; 6.18 (s, 1H) ; 7.25 (d, 1H) ; 7.3-7.7 (m, 8H) ; 8.3 (s, 1H) ; 8.7 (s, 1H) ; 11.1 (s, 1H) ; 11.4 (s, 1H)

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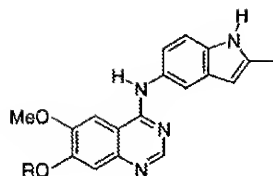
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MS-ESI : 321 [MH]⁺

¹H NMR 溶液: (DMSO-d₆) 2.4 (s, 3H) ; 3.95 (s, 3H) ; 6.12 (s, 1H) ; 7.0 (s, 1H) ; 7.25 (s, 1H) ; 7.7 (s, 1H) ; 7.85 (s, 1H) ; 8.3 (s, 1H) ; 9.35 (s, 1H) ; 10.2 (br s, 1H) ; 10.9 (s, 1H)

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表 XII



実施例 番号	重量 (mg)	収量%	MS-ESI [MH] ⁺	註	R
206	65	41	496	a	
207	62	45		b	

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¹H NMR スペクトル: (DMSO-d₆) 2.0 (m, 2H); 2.4 (s, 3H); 2.7 (t, 2H); 2.95 (m, 4H); 3.15 (m, 4H); 3.95 (s, 3H); 4.2 (t, 2H); 6.15 (s, 1H); 7.18 (s, 1H); 7.28 (m, 2H); 7.7 (s, 1H); 7.85 (s, 1H); 8.35 (s, 1H); 9.4 (s, 1H)

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¹H NMR (400 MHz, CDCl₃): 1.25 (t, 3H); 2.95 (t, 2H); 4.15 (q, 2H); 4.7 (t, 2H); 7.65 (s, 1H); 7.7 (s, 1H).

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^1H NMR λ° CDCl_3 : 2.1-2.2 (m, 3H); 3.65 (m, 2H); 4.6 (t, 2H); 7.6 (s, 1H); 7.72 (s, 1H)

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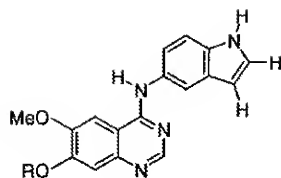
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表 XIII



実施例 番号	重量 (mg)	収量 %	MS-ESI [MH] ⁺	註	R
209	77	57	422	a	
210	64	45	446	b	
211	76	49	482	c	
212	70	48	462	d	
213	85	59	447	e	
214	62	54	365	f	
215	71	54	409	g	
216	73	55	418	h	

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^1H NMR λ° H_2O : (DMSO-d_6) 2.35 (s, 3H) ; 2.68 (t, 2H) ; 2.82 (t, 2H) ; 3.25 (s, 3H) ; 3.5 (t, 2H) ; 3.97 (s, 3H) ; 4.22 (t, 2H), 6.45 (s, 1H) ; 7.18 (s, 1H) ; 7.3-7.45 (m, 3H) ; 7.88 (m, 2H) ; 8.35 (s, 1H) ; 9.42 (s, 1H)

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^1H NMR λ° H_2O : (DMSO-d_6) 2.05 (m, 2H) ; 2.65 (s, 3H) ; 3.6 (t, 2H) ; 3.98 (s, 2H) ; 4.15 (t, 2H) ; 6.45 (s, 1H) ; 7.1 (s, 1H) ; 7.3-7.45 (m, 3H) ; 8.7 (s, 1H) ; 8.8 (s, 1H) ; 8.35 (s, 1H) ; 9.45 (s, 1H)

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^1H NMR λ° H_2O : (CDCl_3) 1.8 (m, 2H) ; 2.52 (t, 1H) ; 2.78 (s, 4H) ; 3.58 (q, 2H) ; 3.7 (t, 2H)

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^1H NMR λ° クト λ : (DMSO- d_6) 2.0 (m, 2H) ; 2.7 (t, 2H) ; 2.95 (br s, 4H) ; 3.15 (br s, 4H) ; 3.97 (s, 3H) ; 4.2 (t, 2H) ; 6.45 (s, 1H) ; 7.2 (s, 1H) ; 7.3-7.5 (m, 3H) ; 7.9 (2s, 2H) ; 8.35 (s, 1H) ; 9.42 (s, 1H)

^1H NMR λ° クト λ : (DMSO- d_6) 2.22 (m, 2H) ; 3.3 (m, 2H) ; 3.65 (s, 3H) ; 3.95 (s, 3H) ; 4.25 (t, 2H) ; 6.45 (s, 1H) ; 7.15 (s, 1H) ; 7.3-7.45 (m, 3H) ; 7.88 (s, 1H) ; 8.0 (s, 1H) ; 8.35 (s, 1H) ; 8.58 (s, 1H) ; 9.45 (s, 1H)

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^1H NMR λ° ʁɪʁ: (CDCl_3) 2.02 (m, 2H) ; 3.45 (t, 2H) ; 3.55 (s, 3H) ; 3.75 (t, 2H) ; 8.15 (s, 1H)

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^1H NMR λ° ʁɪʁ: (DMSO-d_6) 2.0 (m, 2H) ; 2.2 (s, 3H) ; 2.25-2.55 (m, 10H) ; 4.0 (s, 3H) ; 4.2 (t, 2H) ; 6.45 (s, 1H) ; 7.15 (s, 1H) ; 7.35 (m, 2H) ; 7.42 (d, 1H) ; 7.88 (br s, 2H) ; 8.38 (s, 1H) ; 9.42 (s, 1H)

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^1H NMR λ° ʁɪʁ: (DMSO-d_6) 3.4 (s, 3H) ; 3.75 (t, 2H) ; 3.98 (s, 3H) ; 4.38 (t, 2H) ; 6.45 (s, 1H) ; 7.18 (s, 1H) ; 7.35 (m, 2H) ; 7.42 (d, 1H) ; 7.85 (s, 1H) ; 7.9 (s, 1H) ; 8.38 (s, 1H) ; 9.5 (s, 1H)

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^1H NMR λ° 𐀀𐀀𐀀: (DMSO d_6) 3.3 (s, 3H) ; 3.5 (t, 2H) ; 3.65 (t, 2H) ; 3.85 (t, 2H) ; 4.0 (s, 3H) ; 4.28 (t, 2H) ; 6.45 (s, 1H) ; 7.18 (s, 1H) ; 7.35 (m, 2H) ; 7.45 (d, 1H) ; 7.88 (s, 1H) ; 7.9 (s, 1H) ; 8.35 (s, 1H) ; 9.45 (s, 1H)

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^1H NMR λ° 𐀀𐀀𐀀: (DMSO d_6) 1.3-1.6 (m, 6H) ; 2.5 (br s, 4H) ; 2.7 (t, 2H) ; 3.98 (s, 3H) ; 4.25 (t, 2H) ; 6.45 (s, 1H) ; 7.18 (s, 1H) ; 7.35 (m, 2H) ; 7.42 (d, 1H) ; 7.9 (br s, 2H) ; 8.38 (s, 1H) ; 9.42 (s, 1H)

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^1H NMR λ° 𐀀𐀀𐀀: (DMSO d_6) 6.41 (s, 1H) ; 6.6 (dd, 1H) ; 6.63 (s, 1H) ; 7.0 (t, 1H) ; 7.4 (d, 1H) ; 7.87 (br s, 1H)

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MS-ESI : 397 [MH]⁺

¹H NMR 溶液: (DMSO-d₆) 4.02 (s, 3H) ; 5.35 (s, 2H) ; 6.5 (s, 1H) ; 7.25 (dd, 1H) ; 7.35-7.6 (m, 5H) ; 7.63 (d, 1H) ; 7.72 (s, 1H) ; 8.3 (s, 1H) ; 8.75 (s, 1H) ; 11.3 (br s, 1H)

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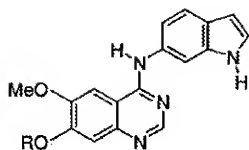
MS-ESI : 307 [MH]⁺

¹H NMR 溶液: (DMSO-d₆) 4.0 (s, 3H) ; 6.4 (s, 1H) ; 7.0 (s, 1H) ; 7.3 (m, 2H) ; 7.5 (d, 1H) ; 7.85 (s, 1H) ; 8.0 (s, 1H) ; 8.35 (s, 1H) ; 9.35 (s, 1H) ; 11.05 (s, 1H)

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表 XIV



実施例 番号	重量 (mg)	収量 %	MS-ESI [MH] ⁺	註	R
217	46	35	416	a	
218	57	37	482	b	
219	37	25	462	c	
220	38	29	418	d	
221	10	7	418	e	
222	94	61	483	f	
223	56	44	398	g	

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^1H NMR λ° H_2O : (DMSO- d_6) 2.42 (t, 2H) ; 4.02 (s, 3H) ; 4.2 (t, 2H) ; 4.62 (t, 2H) ; 6.42 (s, 1H) ; 7.15 (s, 1H) ; 7.3 (m, 2H) ; 7.55 (d, 1H) ; 7.75 (s, 1H) ; 7.92 (s, 1H) ; 8.02 (s, 1H) ; 8.2 (s, 1H) ; 8.42 (s, 1H) ; 9.45 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 2.0 (m, 2H) ; 2.7 (t, 2H) ; 2.95 (br s, 4H) ; 3.12 (br s, 4H) ; 4.0 (s, 3H) ; 4.2 (t, 2H) ; 6.42 (s, 1H) ; 7.2 (s, 1H) ; 7.3 (m, 2H) ; 7.55 (d, 1H) ; 7.9 (s, 1H) ; 8.02 (s, 1H) ; 8.42 (s, 1H) ; 9.48 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 2.22 (t, 2H) ; 3.3 (t, 2H) ; 3.6 (s, 3H) ; 4.0 (s, 3H) ; 4.28 (t, 2H) ; 6.4 (s, 1H) ; 7.18 (s, 1H) ; 7.3 (m, 2H) ; 7.53 (d, 1H) ; 7.9 (s, 1H) ; 8.02 (s, 1H) ; 8.42 (s, 1H) ; 8.58 (s, 1H) ; 9.45 (s, 1H)

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^1H NMR スペクトル: (DMSO-d_6) 1.3-1.6 (m, 6H) ; 2.5 (br s, 4H) ; 2.75 (t, 2H) ;
 4.0 (s, 3H) ; 4.25 (t, 2H) ; 6.42 (s, 1H) ; 7.2 (s, 1H) ; 7.3 (m, 2H) ; 7.55 (d,
 1H) ; 7.9 (s, 1H) ; 8.02 (s, 1H) ; 8.42 (s, 1H) ; 9.45 (s, 1H)

MS-ESI : 130 $[\text{MH}]^+$

^1H NMR スペクトル: (CDCl_3) 1.6-1.8 (m, 6H) ; 2.55 (br s, 4H) ; 2.75 (t, 2H) ;
 3.85 (t, 2H) ; 5.2-5.8 (br s, 1H)

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^1H NMR λ° C_6D_6 : (DMSO- d_6) 2.08 (m, 2H) ; 2.22 (s, 6H) ; 2.95 (s, 3H) ; 3.6 (t, 2H) ; 4.05 (s, 3H) ; 4.15 (t, 2H) ; 6.35 (s, 2H) ; 6.42 (s, 1H) ; 7.15 (s, 1H) ; 7.3 (m, 2H) ; 7.55 (d, 1H) ; 7.92 (s, 1H) ; 8.02 (s, 1H) ; 8.4 (s, 1H) ; 9.45 (s, 1H)

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MS-EI : 194 [M.] $^{+}$

^1H NMR λ° C_6D_6 : (CDCl $_3$) 1.75-1.95 (m, 2H) ; 2.4 (s, 6H) ; 3.0 (s, 3H) ; 3.48 (t, 2H) ; 3.7 (t, 2H) ; 6.25 (s, 2H)

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^1H NMR λ° C_6D_6 : (DMSO- d_6) 4.02 (s, 3H) ; 5.35 (s, 2H) ; 6.42 (s, 1H) ; 7.22-7.4 (m, 3H) ; 7.5 (m, 1H) ; 7.55 (d, 1H) ; 7.95 (s, 1H) ; 7.97 (d, 1H) ; 8.0 (s, 1H) ; 8.42 (s, 1H) ; 8.6 (d, 1H) ; 8.78 (s, 1H) ; 9.5 (s, 1H)

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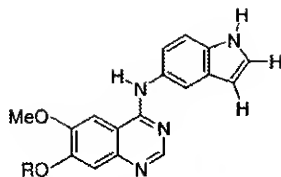
¹H NMR (λ⁸ クロロホルム: (DMSO-d₆) 1.85-2.7 (br s, 4H); 2.95-3.1 (br s, 2H); 3.0 (m, 2H); 3.4-3.5 (m, 2H); 3.8 (d, 2H); 4.0 (s, 3H); 4.8 (d, 2H); 6.0-6.3 (m, 2H); 6.5 (s, 1H); 7.2-7.53 (m, 4H); 7.75 (s, 1H); 8.25 (s, 1H); 8.8 (br s, 1H)

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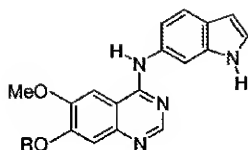
表 XV



実施例 番号	重量 (mg)	収量%	MS-ESI [MH] ⁺	註	R
225	77	50	483	a	

¹H NMR スペクトル: (DMSO-d₆) 2.2 (m, 2H); 2.5 (2br s, 6H); 3.2 (s, 3H); 3.8 (t, 2H); 4.1 (s, 3H); 4.25 (t, 2H); 6.52 (s, 1H); 6.75 (br s, 1H); 6.9 (br s, 1H); 7.35 (dd, 1H); 7.45 (br s, 2H); 7.5 (d, 1H); 7.8 (s, 1H); 8.4 (s, 1H); 8.75 (s, 1H)

表 XVI



実施例 番号	重量 (mg)	収量%	MS-ESI [MH] ⁺	註	R
227	24	17	441	a	
228	14	10	430	b	
229	15	10	447	c	

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¹H NMR スペクトル: (DMSO-d₆) 3.3 (s, 3H) ; 4.0 (s, 3H) ; 4.18 (t, 2H) ; 4.45 (t, 2H) ; 6.5 (s, 1H) ; 7.35 (d, 1H) ; 7.35-7.5 (m, 4H) ; 7.62 (d, 1H) ; 7.75 (s, 1H) ; 8.3 (d, 2H) ; 8.4 (s, 1H) ; 8.75 (s, 1H)

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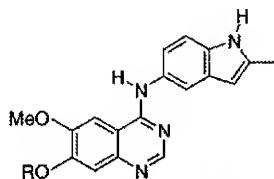
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^1H NMR λ° H_2O : (DMSO- d_6) 1.8-2.1 (m, 4H) ; 2.9-3.1 (m, 2H) ; 3.4-3.5 (br s, 2H) ; 3.87 (d, 2H) ; 4.05 (s, 3H) ; 4.9 (d, 2H) ; 6.1 (m, 1H) ; 6.3 (m, 1H) ; 6.5 (s, 1H) ; 7.25 (d, 1H) ; 7.45 (m, 2H) ; 7.65 (d, 1H) ; 7.75 (s, 1H) ; 8.3 (s, 1H) ; 8.8 (s, 1H)

MS-ESI : 443 [MH] $^+$

^1H NMR λ° H_2O : (DMSO- d_6) 2.42 (s, 3H) ; 2.62 (s, 3H) ; 4.03 (s, 3H) ; 4.3 (t, 2H) ; 4.35 (t, 2H) ; 6.2 (s, 1H) ; 7.22 (d, 1H) ; 7.35 (d, 1H) ; 7.45 (s, 1H) ; 7.6 (dd, 1H) ; 7.65 (dd, 1H) ; 7.7 (s, 1H) ; 8.35 (s, 1H) ; 8.75 (s, 1H)

表 XVII



実施例 番号	重量 (mg)	収量%	MS-ESI [MH] ⁺	註	R
231	49	31	497	a	
232	25	18	444	b	
233	23	15	476	c	
234	33	22	461	d	
235	26	19	423	e	

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^1H NMR スペクトル: (DMSO-d_6) 2.2 (m, 2H) ; 2.4 (s, 6H) ; 2.45 (s, 3H) ; 3.15 (s, 3H) ; 3.75 (t, 2H) ; 4.02 (s, 3H) ; 4.25 (t, 2H) ; 6.2 (s, 1H) ; 6.72 (br s, 1H) ; 6.85 (br s, 1H) ; 7.2 (dd, 1H) ; 7.3-7.4 (m, 2H) ; 7.62 (s, 1H) ; 8.3 (s, 1H) ; 8.7 (s, 1H)

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^1H NMR スペクトル: (DMSO-d_6) 1.8-2.1 (m, 4H) ; 2.4 (s, 3H) ; 2.9-3.1 (m, 2H) ; 3.4-3.6 (m, 2H) ; 3.9 (d, 2H) ; 4.05 (s, 3H) ; 4.9 (d, 2H) ; 6.1 (m, 1H) ; 6.2 (s, 1H) ; 6.3 (d, t, 1H) ; 7.2 (m, 1H) ; 7.37 (d, 1H) ; 7.4 (s, 1H) ; 7.32 (s, 1H) ; 8.3 (s, 1H) ; 8.75 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 2.25 (m, 2H) ; 2.45 (s, 3H) ; 3.35 (t, 2H) ; 3.65 (s, 3H) ; 4.05 (s, 3H) ; 4.35 (t, 2H) ; 6.2 (s, 1H) ; 7.2 (d, 1H) ; 7.35 (s, 1H) ; 7.37 (d, 1H) ; 7.62 (s, 1H) ; 8.25 (s, 1H) ; 8.75 (s, 1H) ; 8.9 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 2.45 (s, 3H) ; 3.28 (s, 3H) ; 3.5 (t, 2H) , 3.65 (t, 2H) ; 3.9 (t, 2H) ; 4.02 (s, 3H) ; 4.33 (t, 2H) ; 6.2 (s, 1H) ; 7.2 (d, 1H) ; 7.4 (m, 2H) ; 7.63 (s, 1H) ; 8.28 (s, 1H) ; 8.73 (s, 1H)

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MS-ESI : 444 [MH]⁺

¹H NMR spectrum (DMSO-d₆, CF₃COOD) 1.7 (m, 2H) ; 2.15 (d, 2H) ; 2.2-2.35 (m, 1H) ; 3.20 (t, 2H) ; 3.65 (d, 2H) ; 4.1 (s, 3H) ; 4.25 (d, 2H) ; 4.62 (s, 2H) ; 6.5 (s, 0.5 H, partly exchanged) ; 7.1 (dd, 1H) ; 7.5 (s, 1H) ; 7.5-7.6 (m, 3H) ; 7.85 (s, 1H) ; 9.1 (s, 1H)

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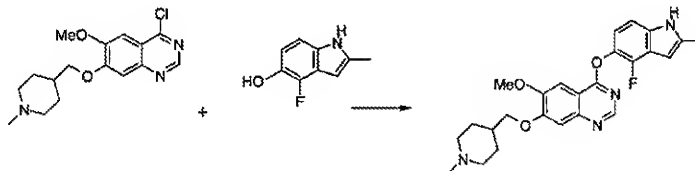
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MS-ESI: 347 [MH]⁺

¹H NMR 測定条件: (DMSO-d₆) 1.42 (m, 2H) ; 1.85 (d, 2H) ; 1.8-1.9 (m, 1H) ;
2.2 (t, 2H) ; 2.85 (d, 2H) ; 3.75 (s, 2H) ; 4.05 (s, 3H) ; 4.15 (d, 2H) ; 7.42 (s,
1H) ; 7.5 (s, 1H) ; 8.9 (s, 1H)



MS-ESI: 451 [MH]⁺

¹H NMR 測定値 (DMSO-d₆) 1.4 (m, 2H); 1.8 (d, 2H); 1.7-1.9 (m, 1H); 1.9 (t, 2H); 2.2 (s, 3H); 2.45 (s, 3H); 2.8 (d, 2H); 4.02 (s, 3H); 4.1 (d, 2H); 6.25 (s, 1H); 7.0 (dd, 1H); 7.2 (d, 1H); 7.4 (s, 1H); 7.62 (s, 1H); 8.5 (s, 1H)

元素分析 : 実測値 C 64.2 H 6.5 N 11.7

C₂₅H₂₇N₃O₃ 0.91 対照 0.08CH₂Cl₂ 0.1H₂O 理論値 C 63.9 H 6.4 N 11.5%

^1H NMR スペクトル: (DMSO-d_6) 3.85 (s, 3H); 6.38 (s, 1H, 6-7位); 6.45 (s, 1H;
4-7位); 6.9-7.4 (m, 3H)

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^1H NMR スペクトル: (DMSO-d_6) 1.65 (s, 9H); 3.9 (s, 3H); 6.6 (d, 1H, 6-7位);
6.72 (d, 1H, 4-7位); 7.2 (t, 1H, 6-7位); 7.4 (d, 1H, 4-7位); 7.62 (d, 1H, 6-
7位); 7.68 (d, 1H, 4-7位); 7.78 (s, 1H, 4-7位); 7.85 (s, 1H, 6-7位)

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6-フルオロ-5-メトキシ-2-メチルイソトール:

MS-ESI: 180 [MH]⁺

¹H NMR スペクトル: (DMSO-d₆) 2.35 (s, 3H); 3.8 (s, 3H); 6.05 (s, 1H); 7.1 (s, 1H); 7.12 (s, 1H); 10.8 (s, 1H)

4-フルオロ-5-メトキシ-2-メチルイソトール:

MS-ESI: 180 [MH]⁺

¹H NMR スペクトル: (DMSO-d₆) 2.35 (s, 3H); 3.8 (s, 3H); 6.15 (s, 1H); 6.9 (t, 1H); 7.05 (d, 1H); 11.0 (s, 1H)

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MS-ESI: 166 [MH]⁺

¹H NMR スペクトル: (DMSO-d₆) 2.35 (s, 3H); 6.05 (s, 1H); 6.65 (dd, 1H); 6.9 (d, 1H); 8.75 (s, 1H); 10.9 (s, 1H)

¹³C NMR スペクトル: (DMSO-d₆) 13.5; 94.0; 106.0; 112; 118.5 (d); 132 (d); 136 (d); 136.5; 142.5 (d)

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[illegible]

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¹H NMR 測定値: (CDCl₃) 2.35 (s, 3H) ; 4.25 (s, 2H) ; 5.25 (s, 2H) ; 7.0 (dd, 1H) ; 7.32-7.5 (m, 5H) ; 8.0 (dd, 1H)

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[illegible]

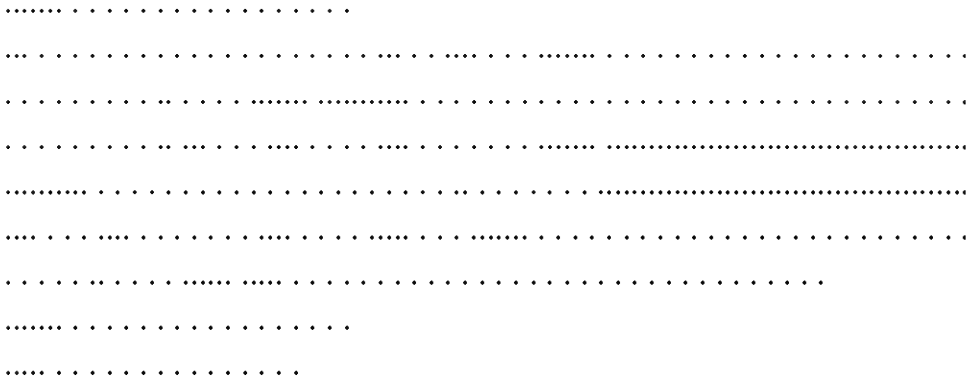
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[illegible]

MS-ESI : 250 [MNa]⁺

¹H NMR 溶液: (CDCl₃) 2.38 (s, 3H) ; 4.0 (s, 3H) ; 4.25 (s, 2H) ; 7.0 (dd, 1H) ; 8.05 (d, 1H)

¹H NMR 溶液: (DMSO) 2.35 (s, 3H) ; 3.8 (s, 3H) ; 6.1 (s, 1H) ; 6.85 (dd, 1H) ; 7.02 (d, 1H)

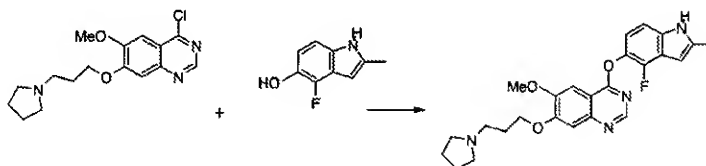


¹H NMR (DMSO-d₆) 1.4 (br s, 2H); 1.5 (m, 4H); 1.95 (m, 2H); 2.25-2.5 (m, 6H); 2.45 (s, 3H); 4.0 (s, 3H); 4.25 (t, 2H); 6.25 (s, 1H); 7.0 (dd, 1H); 7.15 (d, 1H); 7.4 (s, 1H); 7.6 (s, 1H); 8.5 (s, 1H)



MS-ESI: 480 [MH]⁺

¹H NMR 溶液: (DMSO-d₆) 2.0 (t, 2H); 2.15 (s, 3H); 2.45 (s, 3H); 2.2-2.6 (m, 10H); 4.02 (s, 3H); 4.25 (t, 2H); 6.25 (s, 1H); 7.0 (dd, 1H); 7.18 (d, 1H); 7.4 (s, 1H); 7.62 (s, 1H); 8.5 (s, 1H)



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MS-ESI: 451 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.7 (br s, 4H); 2.0 (m, 2H); 2.41 (s, 3H); 2.5 (br s, 4H); 2.6 (t, 2H); 4.0 (s, 3H); 4.25 (t, 2H); 6.25 (s, 1H); 7.0 (dd, 1H); 7.2 (d, 1H); 7.4 (s, 1H); 7.6 (s, 1H); 8.5 (s, 1H)

元素分析 : 実測値 C 63.3 H 6.4 N 11.9

C₂₅H₂₇FN₄O₃ · 1.08 H₂O; 0.16 水分 理論値 C 63.6 H 6.3 N 11.8%

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MS-ESI: 451 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.2-1.3 (m, 2H); 1.4-1.55 (m, 1H); 1.7-1.9 (m, 6H); 2.15 (s, 3H); 2.75 (d, 2H); 4.0 (s, 3H); 4.3 (t, 2H); 6.55 (s, 1H); 7.1 (dd, 1H); 7.3 (d, 1H); 7.4 (s, 1H); 7.5 (s, 1H); 7.6 (s, 1H); 8.5 (s, 1H); 11.5 (s, 1H)

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¹H NMR (λ⁺クル): (CDCl₃) 0.95-1.05 (m, 4H) ; 1.45 (s, 9H) ; 1.4-1.6 (m, 3H) 2.45 (s, 3H) ; 2.62 (t, 2H) ; 3.9-4.1 (m, 2H) ; 4.1 (t, 2H) ; 7.35 (d, 2H) ; 7.8 (d, 2H)

[illegible]

MS-ESI : 540 [MNa]⁺

¹H NMR 溶媒: (CDCl₃) 1.2 (s, 9H) ; 1.15-1.25 (m, 2H) ; 1.48 (s, 9H) ; 1.65-1.75 (m, 1H) ; 1.7 (d, 2H) ; 1.9 (dd, 2H) ; 2.72 (t, 2H) ; 4.0 (s, 3H) ; 4.0-4.2 (m, 2H) ; 4.2 (t, 2H) ; 5.95 (s, 2H) ; 7.1 (s, 1H) ; 7.65 (s, 1H) ; 8.2 (s, 1H)

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¹H NMR 溶媒: (CDCl₃) 1.2 (s, 9H) ; 1.65 (m, 2H) ; 1.9 (br s, 2H) ; 1.8-1.9 (m, 1H) ; 2.0 (d, 2H) ; 2.9 (t, 2H) ; 3.45 (d, 2H) ; 4.0 (s, 3H) ; 4.2 (t, 2H) ; 5.95 (s, 2H) ; 7.1 (s, 1H) ; 7.65 (s, 1H) ; 8.2 (s, 1H)

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MS-ESI: 432 [MH]⁺

¹H NMR λ^Λ ʁɪʁ: (CDCl₃) 1.22 (s, 9H) ; 1.68 (br s, 3H) ; 1.9 (m, 4H) ; 2.32 (br s, 2H) ; 2.52 (s, 3H) ; 3.18 (d, 2H) ; 4.0 (s, 3H) ; 4.2 (t, 2H) ; 5.95 (s, 2H) ; 7.1 (s, 1H) ; 7.65 (s, 1H) ; 8.2 (s, 2H)

MS-ESI: 318 [MH]⁺

¹H NMR λ^Λ ʁɪʁ: (DMSO-d₆) 1.3 (m, 2H) ; 1.58 (br s, 1H) ; 1.72 (dd, 2H) ; 1.8 (d, 2H) ; 2.4 (s, 3H) ; 2.2-2.45 (m, 2H) ; 3.0 (br s, 2H) ; 3.85 (s, 3H) ; 4.15 (t, 2H) ; 7.15 (s, 1H) ; 7.45 (s, 1H) ; 8.0 (s, 1H)

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MS-ESI : 336 [MH]⁺

¹H NMR 溶媒: (CDCl₃) 1.4-1.7 (m, 3H) ; 1.8 (d, 2H) ; 1.9 (dd, 2H) ; 2.05 (t, 2H) ; 2.35 (s, 3H) ; 2.95 (d, 2H) ; 4.05 (s, 3H) ; 4.25 (t, 2H) ; 7.3 (s, 1H) ; 7.4 (s, 1H) ; 8.88 (s, 1H)

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MS-ESI : 437 [MH]⁺

¹H NMR 溶媒: (DMSO-d₆) 1.3-1.45 (m, 2H) ; 1.8 (d, 2H) ; 1.9 (t, 2H) ; 1.7-1.9 (m, 1H) ; 2.17 (s, 3H) ; 2.8 (d, 2H) ; 4.0 (s, 3H) ; 4.1 (d, 2H) ; 6.48 (br s, 1H) ; 7.38 (d, 1H) ; 7.4 (s, 1H) ; 7.42 (t, 1H) ; 7.58 (d, 1H) ; 7.6 (s, 1H) ; 8.5 (s, 1H)

元素分析	実測値	C	65.0	H	5.8	N	12.7
C ₂₄ H ₂₅ FN ₄ O ₃ · 0.4 H ₂ O	理論値	C	65.0	H	5.9	N	12.6%

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^1H NMR スペクトル: (CDCl_3) 5.3 (s, 2H); 7.1 (t, 1H); 7.35-7.55 (m, 5H); 8.0 (m, 2H)

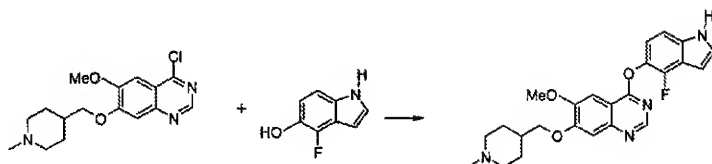
^1H NMR スペクトル: (DMSO-d_6) 4.22 (s, 2H, 3-シノノヒサキシ性体); 4.3 (s, 2H, 5-シノノヒサキシ性体); 5.32 (s, 2H, 5-シノノヒサキシ性体); 5.36 (s, 2H, 3-シノノヒサキシ性体); 7.3-7.7 (m, 6H); 8.1 (d, 1H, 3-シノノヒサキシ性体); 8.2 (d, 1H, 5-シノノヒサキシ性体)

4-フルオロ-5-ヒト'ロキシント'ール:

^1H NMR スペクトル: (DMSO-d_6) 6.32 (s, 1H) ; 6.75 (dd, 1H) ; 7.0 (d, 1H) ; 7.28 (dd, 1H) ; 8.8 (br s, 1H) ; 11.05 (br s, 1H)

6-フルオロ-5-ヒト'ロキシント'ール:

^1H NMR スペクトル: (DMSO-d_6) 6.25 (s, 1H) ; 7.0 (d, 1H) ; 7.12 (d, 1H) ; 7.2 (dd, 1H) ; 9.0 (br s, 1H)



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MS - ESI : 437 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.3-1.5 (m, 2H) ; 1.8 (d, 2H) ; 1.9 (t, 2H) ; 1.7-1.95 (m, 1H) ; 2.2 (s, 3H) ; 2.8 (d, 2H) ; 4.02 (s, 3H) ; 4.1 (d, 2H) ; 6.55 (s, 1H) ; 7.1 (t, 1H) ; 7.3 (d, 1H) ; 7.4 (s, 1H) ; 7.48 (t, 1H) ; 7.62 (s, 1H) ; 8.5 (s, 1H)

元素分析	実測値	C	64.8	H	5.8	N	12.6
C ₂₄ H ₂₃ FN ₄ O ₃ 0.4 H ₂ O	理論値	C	65.0	H	5.9	N	12.6%

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MS-ESI : 466 [MH]⁺

¹H NMR 測定値: (DMSO-d₆, CF₃COOD) 2.3-2.4 (m, 2H) ; 3.0 (s, 3H) ; 3.2-3.9 (m, 8H) ; 3.5 (t, 2H) ; 4.1 (s, 3H) ; 4.4 (t, 2H) ; 6.52 (d, 1H) ; 7.45 (d, 1H) ; 7.48 (s, 1H) ; 7.6 (s, 1H) ; 7.65 (d, 1H) ; 7.82 (s, 1H) ; 9.0 (s, 1H)

元素分析	実測値	C	62.1	H	6.4	N	14.2
C ₂₅ H ₂₈ FN ₅ O ₃ 0.9 H ₂ O	理論値	C	62.3	H	6.2	N	14.5%

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MS-ESI : 427-429 [MH]⁺

¹H NMR 測定条件: (DMSO-d₆) 1.18 (s, 9H) ; 2.32 (m, 2H) ; 3.7 (t, 2H) ; 3.92 (s, 3H) ; 4.28 (t, 2H) ; 5.95 (s, 2H) ; 7.2 (s, 1H) ; 7.5 (s, 1H) ; 8.4 (s, 1H)

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MS-ESI : 447 [MH]⁺

¹H NMR 測定条件: (DMSO-d₆, CF₃COOD) 1.15 (s, 9H) ; 2.25 (t, 2H) ; 2.5 (s, 3H) ; 3.45 (t, 2H) ; 3.2-4.0 (m, 8H); 3.9 (s, 3H) ; 4.25 (t, 2H) ; 5.95 (s, 2H) ; 7.22 (s, 1H) ; 7.55 (s, 1H) ; 8.6 (s, 1H)

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MS-ESI : 333 [MH]⁺

¹H NMR 測定条件: (DMSO-d₆) 1.92 (m, 2H) ; 2.15 (s, 3H) ; 2.2-2.5 (m, 10H) ; 3.88 (s, 3H) ; 4.15 (t, 2H) ; 7.1 (s, 1H) ; 7.45 (s, 1H) ; 7.98 (s, 1H)

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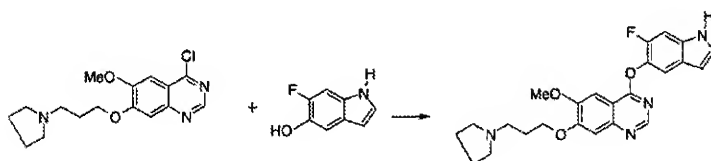
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MS-ESI : 351-353 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.98 (t, 2H) ; 2.18 (s, 3H) ; 2.45 (t, 2H) ; 2.22-2.5 (m, 8H) ; 4.05 (s, 3H) ; 4.28 (t, 2H) ; 7.4 (s, 3H) ; 7.45 (s, 1H) ; 8.9 (s, 1H)



MS-ESI : 437 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.7-1.8 (m, 4H) ; 2.0-2.1 (m, 2H) ; 2.48 (br s, 4H) ; 2.6 (t, 2H) ; 4.02 (s, 3H) ; 4.3 (t, 2H) ; 6.5 (s, 1H) ; 7.4 (d, 1H) ; 7.4 (s, 1H) ; 7.45 (t, 1H) ; 7.6 (d, 1H) ; 7.62 (s, 1H) ; 8.52 (s, 1H)

元素分析	実測値	C	65.4	H	6.0	N	12.9
C ₂₈ H ₂₅ N ₃ O ₃ · 0.2 H ₂ O	理論値	C	65.5	H	5.8	N	12.7%

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MS-ESI : 532 [MH]⁺

¹H NMR スペクトル: (DMSO-d₆) 1.3-1.45 (m, 2H) ; 1.8 (d, 2H) ; 1.7-1.9 (m, 1H) ;
2.0 (t, 2H) ; 2.3-2.45 (m, 8H) ; 2.4 (s, 3H) ; 2.95 (d, 2H) ; 3.6 (t, 4H) ; 4.0 (s,
3H) ; 4.08 (d, 2H) ; 6.18 (s, 1H) ; 6.9 (dd, 1H) ; 7.3 (s, 1H) ; 7.35 (d, 1H) ; 7.4
(s, 1H) ; 7.6 (s, 1H) ; 8.5 (s, 1H) ; 11.05 (s, 1H)

元素分析

実測値 C 65.3 H 7.1 N 12.6

C₃₀H₃₇N₅O₄ 0.6 H₂O 0.6 計算値

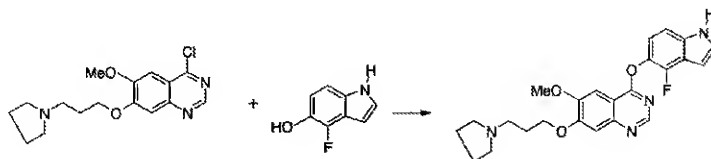
理論値 C 65.4 H 7.3 N 12.5%

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MS-ESI : 437 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.7 (br s, 4H) ; 2.0 (m, 2H) ; 2.45 (br s, 4H) ; 2.6 (t, 2H) ; 4.05 (s, 3H) ; 4.28 (t, 2H) ; 6.58 (s, 1H) ; 7.1 (t, 2H) ; 7.35 (d, 1H) ; 7.4 (s, 1H) ; 7.5 (t, 1H) ; 7.65 (s, 1H) ; 8.52 (s, 1H)

元素分析

測定値 C 65.3 H 5.9 N 12.6

C₂₄H₂₅FN₄O₃ 0.19 水分, 0.17 H₂O

理論値 C 65.2 H 5.9 N 12.6%

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MS-ESI : 451 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.35-1.45 (m, 2H) ; 1.45-1.6 (m, 4H) ; 2.0 (m, 2H) ; 2.35 (br s, 4H) ; 2.42 (t, 2H) ; 4.05 (s, 3H) ; 4.25 (t, 2H) ; 6.5 (s, 1H) ; 7.4 (d, 1H) ; 7.42 (s, 1H) ; 7.44 (t, 1H) ; 7.6 (d, 1H) ; 7.65 (s, 1H) ; 8.5 (s, 1H)

元素分析

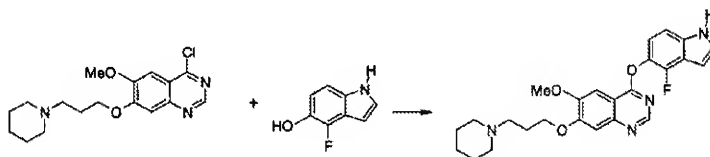
実測値

C 65.9 H 6.2 N 12.3

C₂₅H₂₇FN₄O₃ 0.3 H₂O

理論値

C 65.9 H 6.1 N 12.3%



MS-ESI: 451 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.35-1.45 (m, 2H); 1.55 (m, 4H); 2.0 (m, 2H);
2.38 (br s, 4H); 2.45 (t, 2H); 4.02 (s, 3H); 4.25 (t, 2H); 6.55 (s, 1H); 7.12
(dd, 1H); 7.32 (d, 1H); 7.4 (s, 1H); 7.5 (s, 1H); 7.65 (s, 1H); 8.52 (s, 1H)

元素分析	実測値	C	66.0	H	6.2	N	12.4
C ₂₅ H ₂₇ N ₄ O ₃ · 0.2 H ₂ O	理論値	C	66.1	H	6.1	N	12.3%

MS-ESI: 451 [MH]⁺

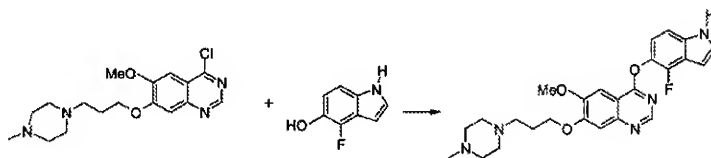
¹H NMR 測定値: (DMSO-d₆) 1.65-1.8 (br s, 4H); 2.02 (m, 2H); 2.4 (s, 3H);
2.48 (br s, 4H); 2.6 (t, 2H); 4.02 (s, 3H); 4.3 (t, 2H); 6.18 (s, 1H); 7.25 (d,
1H); 7.4 (s, 1H); 7.45 (d, 1H); 7.6 (s, 1H); 8.5 (s, 1H)

元素分析	実測値	C	65.6	H	6.1	N	12.2
C ₂₅ H ₂₇ N ₄ O ₃ · 0.4 H ₂ O	理論値	C	65.6	H	6.1	N	12.2%

MS-ESI: 166 [MH]⁺

¹H NMR λ[°] 7.1: (DMSO-d₆) 2.3 (s, 3H) ; 5.95 (s, 1H) ; 6.9 (d, 1H) ; 7.0 (d, 1H) ; 8.85 (s, 1H) ; 10.6 (s, 1H)

¹³C NMR λ[°] 7.1: (DMSO-d₆) 13.3 ; 97.4 (d) ; 98.3 ; 105.5 ; 124.5 ; 128.8 (d) ; 135.6 ; 138.5 (d) ; 148.3 (d).



MS-ESI: 466 [MH]⁺

¹H NMR 測定値: (DMSO-d₆, CF₃COOD) 2.3-2.4 (m, 2H); 2.97 (s, 3H); 3.2-4.1 (m, 8H); 3.5 (t, 2H); 4.07 (s, 3H); 4.4 (t, 2H); 6.6 (d, 1H); 7.15 (t, 1H); 7.38 (d, 1H); 7.5 (d, 1H); 7.6 (s, 1H); 7.82 (s, 1H); 8.95 (s, 1H)

元素分析	実測値	C	64.4	H	6.1	N	15.0
C ₂₅ H ₂₈ N ₅ O ₃	理論値	C	64.5	H	6.1	N	15.0%

MS-ESI: 516 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.3-1.5 (m, 2H); 1.6-1.75 (m, 4H); 1.8 (d, 2H); 1.7-1.9 (m, 1H); 1.95 (t, 2H); 2.45 (s, 3H); 2.4-2.5 (m, 5H); 2.95 (d, 2H); 3.35 (d, 2H); 4.0 (s, 3H); 4.1 (d, 2H); 6.18 (s, 1H); 6.9 (d, 1H); 7.25 (s, 1H); 7.35 (d, 1H); 7.38 (s, 1H); 7.6 (s, 1H); 8.5 (s, 1H); 11.05 (s, 1H)

元素分析	実測値	C	68.6	H	7.2	N	13.3
C ₃₀ H ₃₇ N ₅ O ₃ 0.5 H ₂ O	理論値	C	68.7	H	7.3	N	13.4%

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MS-ESI : 453 [MH]⁺

¹H NMR 測定値: (DMSO-d₆) 1.95-2.05 (m, 2H) ; 2.45 (br s, 4H) ; 2.5 (t, 2H) ;
3.62 (t, 4H) ; 4.02 (s, 3H) ; 4.3 (t, 2H) ; 6.5 (s, 1H) ; 7.4 (d, 1H) ; 7.45 (s, 1H) ;
7.47 (t, 1H) ; 7.58 (d, 1H) ; 7.62 (s, 1H) ; 8.5 (s, 1H)

元素分析	実測値	C	61.6	H	5.5	N	11.9
C ₂₄ H ₂₈ FN ₄ O ₄ · 0.8 H ₂ O	理論値	C	61.7	H	5.7	N	12.0%

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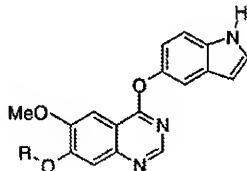
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MS-ESI: 421 [MH]⁺

¹H NMR 測定値: (DMSO-d₆, CF₃COOD) 3.30 (t, 2H); 3.65 (d, 2H); 3.7-3.8 (m, 4H); 4.05 (d, 2H); 4.1 (s, 3H); 4.7 (t, 2H); 6.5 (s, 1H); 7.05 (dd, 1H); 7.4-7.6 (m, 3H); 7.65 (s, 1H); 7.82 (s, 1H); 9.0 (s, 1H)

表 XVIII



実施例 番号	重量 (mg)	収量%	MS-ESI [MH] ⁺	R	註
255	123	51	405		a
256	124	48	434		b
257	165	62	448		c

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^1H NMR λ° DMSO-d_6 : 1.72 (br s, 4H) ; 2.6 (br s, 4H) ; 2.9 (t, 2H) ; 4.0 (s, 3H) ; 4.3 (t, 2H) ; 6.48 (s, 1H) ; 7.0 (dd, 1H) ; 7.4-7.5 (m, 3H) ; 7.6 (s, 1H) ; 8.5 (s, 1H) ; 11.3 (br s, 1H)

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^1H NMR λ° DMSO-d_6 , CF_3COOD : 2.5 (s, 3H) ; 3.35 (t, 2H) ; 3.65 (d, 2H) ; 3.7-3.8 (m, 4H) ; 4.05 (d, 2H) ; 4.1 (s, 3H) ; 4.7 (t, 2H) ; 7.05 (dd, 1H) ; 7.45 (s, 1H) ; 7.5-7.6 (m, 2H) ; 7.65 (s, 1H) ; 7.82 (s, 1H) ; 9.0 (s, 1H)

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^1H NMR λ° CDCl_3 : 2.18(s, 3H); 2.3-2.7(br m, 8H); 2.56(t, 2H); 3.61(t, 2H)

MS - ESI: 145 $[\text{MH}]^+$

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^1H NMR λ° CDCl_3 : 2.15 (s, 3H) ; 2.3-2.4 (br s, 4H) ; 2.5-2.6 (m, 4H) ; 2.8 (t, 2H) ; 4.0 (s, 3H) ; 4.35 (t, 2H) ; 6.45 (s, 1H) ; 7.0 (dd, 1H) ; 7.4-7.5 (m, 4H) ; 7.62 (s, 1H) ; 8.5 (s, 1H)

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MS-ESI : 467 [MH]⁺

¹H NMR 溶液: (DMSO-d₆, CF₃COOD) 1.85-2.0 (m, 2H) ; 2.0-2.15 (m, 2H) ;
2.42 (s, 3H) ; 3.15 (m, 2H) ; 3.4 (d, 2H) ; 3.65 (m, 2H) ; 4.1 (s, 3H) ; 4.32 (d,
2H) ; 4.4 (m, 1H) ; 7.05 (dd, 1H) ; 7.22 (d, 1H) ; 7.6 (s, 1H) ; 7.85 (s, 1H) ;
9.02 (s, 1H)

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MS-ESI : 363 [MH]⁺

¹H NMR 溶液: (DMSO-d₆) 1.12 (s, 9H) ; 2.75 (m, 1H) ; 2.9 (t, 1H) ; 3.4 (m,
1H) ; 3.93 (s, 3H) ; 4.0 (dd, 1H) ; 4.52 (dd, 1H) ; 5.9 (s, 2H) ; 7.2 (s, 1H) ; 7.52
(s, 1H) ; 8.35 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6) 1.15 (s, 9H) ; 1.7 (br s, 4H) ; 2.48 (m, 1H) ; 2.5 (br s, 4H) ; 2.65 (dd, 1H) ; 3.9 (s, 3H) ; 4.0 (br s, 1H) ; 4.05 (dd, 1H) ; 4.18 (dd, 1H) ; 4.95 (br s, 1H) ; 5.9 (s, 2H) ; 7.2 (s, 1H) ; 7.5 (s, 1H) ; 8.35 (s, 1H)

^1H NMR λ° H_2O : (DMSO- d_6 , CF_3COOD) 1.92 (m, 2H) ; 2.05 (m, 2H) ; 3.15 (m, 2H) ; 3.35 (d, 2H) ; 3.62 (m, 2H) ; 3.98 (s, 3H) ; 4.18 (d, 2H) ; 4.32 (m, 1H) ; 7.35 (s, 1H) ; 7.6 (s, 1H) ; 9.2 (s, 1H)

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MS-ESI : 362 [MH]⁺

¹H NMR λ^α ʒ ʒ ʒ: (DMSO_d₆) 1.7 (br s, 4H) ; 2.05 (s, 3H) ; 2.5 (br s, 4H) ; 2.72 (m, 2H) ; 3.9 (s, 3H) ; 4.3 (m, 2H) ; 5.25 (m, 1H) ; 7.2 (s, 1H) ; 7.45 (s, 1H) ; 8.0 (s, 1H)

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¹H NMR λ^α ʒ ʒ ʒ: (DMSO_d₆) 1.7 (br s, 4H) ; 2.05 (s, 3H) ; 2.55 (br s, 4H) ; 2.75 (br s, 2H) ; 4.02 (s, 3H) ; 4.35-4.5 (m, 2H) ; 5.3 (m, 1H) ; 7.4 (s, 1H) ; 7.5 (s, 1H) ; 7.9 (s, 1H)

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^1H NMR λ° C_6H_5 : (DMSO-d_6) 1.7 (br s, 4H) ; 2.05 (s, 3H) ; 2.4 (s, 3H) ; 2.52 (br s, 4H) ; 2.65-2.82 (m, 2H) ; 4.0 (s, 3H) ; 4.4 (m, 2H) ; 5.3 (m, 1H) ; 6.25 (s, 1H) ; 7.0 (dd, 1H) ; 7.18 (d, 1H) ; 7.48 (s, 1H) ; 7.62 (s, 1H) ; 8.5 (s, 1H)

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MS - ESI : 418 $[\text{MH}]^+$

^1H NMR λ° C_6H_5 : (DMSO-d_6 , CF_3COOD) 1.9 (m, 2H) ; 2.05 (m, 2H) ; 2.3 (m, 2H) ; 3.1 (m, 2H) ; 3.4 (t, 2H) ; 3.65 (m, 2H) ; 4.05 (s, 3H) ; 4.35 (t, 2H) ; 6.5 (s, 0.5H, partly exchanged) ; 7.3 (d, 1H) ; 7.4 (s, 1H) ; 7.45 (s, 1H) ; 7.55 (d, 1H) ; 7.8 (s, 1H) ; 8.25 (s, 1H) ; 8.8 (s, 1H)

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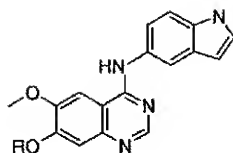
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表 XIX



実施例 番号	重量 (mg)	収量 (%)	MS-ESI [MH] ⁺	註	R
260	101	76	510	a	
261	92	83	418	b	
262	92	80	434	c	
263	84	80	427	d	
264	78	79	401	e	
265	72	70	416	f	

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^1H NMR λ° H_2O : (DMSO- d_6) 1.65-1.8 (m, 2H) ; 2.05 (d, 2H) ; 2.2 (br s, 1H) ;
3.1 (br s, 2H) ; 3.2 (s, 3H) ; 3.5 (br s, 2H) ; 3.6 (d, 2H) ; 3.8 (m, 2H) ; 4.05 (s,
3H) ; 4.1 (d, 2H) ; 6.5 (s, 1H) ; 7.3 (d, 1H) ; 7.42 (m, 2H) ; 7.5 (d, 1H) ; 7.8 (s,
1H) ; 8.4 (s, 1H) ; 8.7 (s, 1H) ; 11.15 (br s, 1H) ; 11.32 (s, 1H) . 11.5 (s, 1H).

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^1H NMR λ° H_2O : (DMSO- d_6) 1.6-1.8 (m, 2H) ; 2.02 (d, 2H) ; 2.15 (br s, 1H) ;
2.75 (s, 3H) ; 3.0 (br s, 2H) ; 3.45 (d, 2H) ; 4.02 (s, 3H) ; 4.1 (d, 2H) ; 6.5 (s,
1H) ; 7.3 (d, 1H) ; 7.4 (m, 2H) ; 7.5 (d, 1H) ; 7.8 (s, 1H) ; 8.3 (s, 1H) ; 8.7 (s,
1H) ; 10.4 (br s, 1H) ; 11.3 (s, 1H)

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^1H NMR λ° H_2O : (DMSO- d_6 ; CF_3COOD) : 2.35 (m, 2H) ; 3.15 (t, 2H) ; 3.3 (t,
2H) ; 3.57 (d, 2H) ; 3.8 (m, 2H) ; 4.02 (d, 2H) ; 4.03 (s, 3H) ; 4.3 (t, 2H) ; 6.5
(d, 1H) ; 7.3 (dd, 1H) ; 7.4 (s, 1H) ; 7.45 (s, 1H) ; 7.52 (d, 1H) ; 7.8 (s, 1H) ;
8.25 (s, 1H) ; 8.78 (s, 1H)

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^1H NMR λ° CF_3COOD : (DMSO- d_6 , CF_3COOD) 2.2-2.4 (m, 2H) ; 3.07 (s, 3H) ; 3.35 (t, 2H) ; 4.05 (s, 3H) ; 4.35 (t, 2H) ; 6.5 (d, 0.5 H, partly exchanged) ; 7.2-7.35 (m, 2H) ; 7.45 (s, 1H) ; 7.5 (d, 1H) ; 7.8 (s, 1H) ; 8.2 (s, 1H) ; 8.75 (s, 1H)

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^1H NMR λ° CF_3COOD : (DMSO- d_6 , CF_3COOD) 4.03 (s, 3H) ; 4.65 (t, 2H) ; 4.8 (t, 2H) ; 6.5 (d, 1H, partly exchanged) ; 7.30 (d, 1H) ; 7.4 (s, 1H) ; 7.45 (s, 1H) ; 7.52 (d, 1H) ; 7.75 (s, 1H) ; 7.8 (s, 1H) ; 7.9 (s, 1H) ; 8.25 (s, 1H) ; 8.75 (s, 1H) ; 9.25 (s, 1H)

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^1H NMR λ° クト λ : (CDCl_3) 1.19(s, 9H); 3.98(s, 3H); 4.34(m, 2H); 4.45(m, 2H); 5.94(s, 2H); 7.02(s, 1H); 7.07(s, 1H); 7.11(s, 1H); 7.64(s, 1H); 7.67(s, 1H); 8.17(s, 1H)

MS - ESI: 423 $[\text{MNa}]^+$

元素分析	:	実測値	C 58.3	H 6.4	N 13.9
$\text{C}_{20}\text{H}_{24}\text{N}_4\text{O}_5 \cdot 0.7\text{H}_2\text{O}$		理論値	C 58.2	H 6.2	N 13.6%

^1H NMR λ° クト λ : (DMSO-d_6) 3.89(s, 3H); 4.4-4.5(m, 4H); 6.9(s, 1H); 7.16(s, 1H); 7.28(s, 1H); 7.47(s, 1H); 7.7(s, 1H); 7.99(s, 1H)

MS - ESI: 287 $[\text{MH}]^+$

元素分析	:	実測値	C 57.8	H 5.2	N 19.3
$\text{C}_{14}\text{H}_{14}\text{N}_4\text{O}_3 \cdot 0.3\text{H}_2\text{O}$		理論値	C 57.7	H 5.1	N 19.2%

^1H NMR λ^{\wedge} H_2O : (DMSO- d_6) 4.01(s, 3H); 4.47(m, 2H); 4.53(m, 2H); 6.89(s, 1H); 7.27(s, 1H); 7.41(s, 1H); 7.49(s, 1H); 7.70(s, 1H); 8.88(s, 1H)
MS - ESI: 327 [MNa] $^+$

^1H NMR λ^{\wedge} H_2O : (DMSO- d_6 , CF_3COOD) 2.5 (m, 2H) ; 4.0 (s, 3H) ; 4.3 (t, 2H) ; 4.6 (t, 2H) ; 6.52 (d, 0.5H partly exchanged) ; 7.3 (s, 1H) ; 7.35 (d, 1H) ; 7.45 (s, 1H) ; 7.55 (d, 1H) ; 7.8 (s, 1H) ; 8.16 (s, 1H) ; 8.66 (s, 1H) ; 8.77 (s, 1H) ; 9.43 (s, 1H)

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^1H NMR λ° クトル: (DMSO- d_6) 1.37(m, 2H); 1.49(m, 4H); 1.96(m, 2H); 2.34(m, 4H); 2.43(t, 2H); 4.00(s, 3H); 4.23(t, 2H); 7.38(s, 1H); 7.62(s, 1H); 7.69(dd, 1H); 8.00(d, 1H); 8.12(d, 1H); 8.34(dd, 1H); 8.54(s, 1H); 8.98(d, 1H)
MS (ESI): 463 (MH) $^+$

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^1H NMR λ° クトル: (DMSO- d_6) 1.90(m, 2H); 2.00(m, 2H); 2.27(m, 2H); 3.02(m, 2H); 3.32(m, 2H); 3.59(m, 2H); 4.00(s, 3H); 4.33(t, 2H); 7.43(s, 1H); 7.62(s, 1H); 7.70(dd, 1H); 7.99(d, 1H); 8.11(d, 1H); 8.35(dd, 1H); 8.54(s, 1H); 8.97(d, 1H)
MS (ESI): 449 (MH) $^+$

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m. p. 250 – 251°C

^1H NMR δ (DMSO- d_6) 1.66 (m, 1H), 2.10 (m, 2H), 2.40 (s, 3H), 2.50 (m, 2H), 2.84 (s, 3H), 3.34 (m, 2H), 3.99 (s, 3H), 4.12 (d, 2H), 6.12 (s, 1H), 6.86 (m, 1H), (d, 1H), 7.30 (d, 1H), 7.38 (s, 1H), 7.59 (s, 1H), 8.48 (s, 1H)および 10.98 (br s, 1H).

MS (ESI) : 447 (MH) $^+$

元素分析	実測値	C	66.8	H	5.9	N	12.4
$\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_4 \cdot 0.2 \text{H}_2\text{O}$	理論値	C	66.7	H	5.9	N	12.5%

^1H NMR スペクトル: (DMSO- d_6) 2.10 (s, 3H), 2.4 (m, 13H), 3.98 (s, 3H), 4.06 (m, 3H), 4.90 (br s, 1H), 6.12 (s, 1H), 6.85 (dd, 1H), 7.3 (m, 2H), 7.58 (s, 1H), 8.42 (s, 1H) および 10.98 (br s, 1H)

MS (ESI): 478 (MH)⁺

元素分析

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実測値 C 61.3 H 6.3 N 13.8

$\text{C}_{26}\text{H}_{30}\text{N}_4\text{O}_4 \cdot 0.2\text{H}_2\text{O} \cdot 0.5$ ジクロロメタン

理論値 C 61.9 H 6.2 N 13.4%

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¹H NMR スペクトル: (DMSO-d₆) 2.40 (s, 3H), 2.75 (m, 1H), 2.90 (m, 1H), 3.40 (m, 1H), 3.98 (s, 3H), 4.05 (m, 1H), 4.60 (m, 1H), 6.15 (s, 1H), 6.85 (dd, 1H), 7.30 (m, 2H) 7.40 (s, 1H), 7.60 (s, 1H), 8.45 (s, 1H)および 10.98 (s, 1H)
MS (ESI): 378 (MH)⁺

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^1H NMR スペクトル: (DMSO- d_6) 0.95 (t, 6H), 2.10 (s, 3H), 2.4 (m, 6H), 3.98 (s, 3H), 4.14 (m, 3H), 4.84 (br s, 1H), 6.12 (s, 1H), 6.85 (dd, 1H), 7.3 (m, 3H), 7.58 (s, 1H), 8.42 (s, 1H)および10.98 (br s, 1H)

MS (ESI): 448 (MH)⁺

元素分析 : 実測値 C 64.3 H 6.6 N 12.0

$\text{C}_{25}\text{H}_{30}\text{N}_4\text{O}_4 \cdot 0.4$ シクロクサントン 理論値 C 64.0 H 6.4 N 11.6%

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^1H NMR スペクトル: (DMSO- d_6) 2.20 (s, 3H), 3.98 (s, 3H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.20 (s, 1H), 7.35 (m, 3H), 7.58 (s, 1H), 8.40 (s, 1H)および10.82 (br s, 1H)

MS (ESI): 322 (MH)⁺

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¹H NMR λ⁺ 412 (CDCl₃) 2.30 (s, 3H), 4.10 (s, 3H), 5.36 (s, 2H), 7.04 (m, 2H), 7.43 (m, 8H), 7.62 (s, 1H), 8.02 (s, 1H), および 8.60 (s, 1H)
MS (ESI) : 412 (MH)⁺

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^1H NMR スペクトル: (DMSO- d_6) 1.98 (m, 2H), 2.20 (s, 3H), 2.40 (t, 4H), 2.50 (m, 2H), 3.60 (t, 4H), 3.98 (s, 3H), 4.20 (t, 2H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.35 (m, 3H), 7.60 (s, 1H), 8.45 (s, 1H), および 10.82 (br s, 1H)

MS (ESI): 449 (MH)⁺

元素分析	:	実測値	C	64.2	H	6.0	N	11.8
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_4 \cdot 0.7\text{H}_2\text{O} \cdot 0.7$ イタリル		理論値	C	64.2	H	6.9	N	11.4%

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^1H NMR スペクトル: (DMSO- d_6) 2.20 (s, 3H), 2.55 (t, 4H), 2.80 (t, 2H), 3.60 (t, 4H), 3.98 (s, 3H), 4.30 (t, 2H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.35 (m, 2H), 7.40 (s, 1H), 7.60 (s, 1H), 8.45 (s, 1H), および 10.82 (br s, 1H)

MS (ESI): 449 (MH)⁺

元素分析	:	実測値	C	64.1	H	6.3	N	12.2
$\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_4 \cdot 0.4\text{H}_2\text{O} \cdot 0.8$ イタリル		理論値	C	64.3	H	6.1	N	11.7%

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¹H NMR スペクトル: (DMSO-d₆) 1.3 (m, 4H), 1.42 (s, 9H), 1.90 (d, 2H), 2.10 (m, 1H), 2.28 (s, 3H), 2.80 (m, 2H), 3.98 (s, 3H), 4.08 (d, 2H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.35 (m, 3H), 7.60 (s, 1H), 8.45 (s, 1H), および 10.82 (br s, 1H)
MS (ESI) : 519 (MH)⁺

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^1H NMR スペクトル: (DMSO- d_6) 1.98 (m, 2H), 2.17 (s, 3H), 2.65 (t, 2H), 2.90 (t, 4H), 3.10 (t, 4H), 3.98 (s, 3H), 4.25 (t, 2H), 6.95 (dd, 1H), 7.15 (s, 1H), 7.30 (d, 1H), 7.35 (m, 2H), 7.60 (s, 1H), 8.45 (s, 1H), および 10.82 (br s, 1H)

MS (ESI): 497 (MH)⁺

元素分析	:	実測値	C	58.4	H	5.5	N	11.1
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_5\text{S} \cdot 0.8\text{H}_2\text{O}$		理論値	C	58.8	H	5.8	N	11.0%

^1H NMR スペクトル: (DMSO- d_6) 1.35 (m, 2H), 1.80 (m, 2H), 2.05 (m, 1H), 2.10 (s, 3H), 2.70 (m, 2H), 3.10 (m, 2H), 3.98 (s, 3H), 4.05 (d, 2H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.34 (m, 3H), 7.60 (s, 1H), 8.45 (s, 1H), および 10.82 (br s, 1H)

MS (ESI): 419 (MH)⁺

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MS (ESI) : 458 (MH)⁺

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^1H NMR スペクトル: (DMSO- d_6) 2.20 (s, 3H), 2.80 (m, 1H), 2.90 (m, 1H), 3.42 (m, 1H), 3.98 (s, 3H), 4.02 (m, 1H), 4.60 (m, 1H), 6.98 (dd, 1H), 7.18 (s, 1H) 7.35 (m, 3H), 7.60 (s, 1H), 8.45 (s, 1H)および 10.82 (s, 1H)

MS (ESI): 378 (MH) $^+$

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^1H NMR スペクトル: (DMSO- d_6) 1.38 (m, 2H), 1.50 (m, 4H), 2.34 (m, 9H), 3.98 (s, 3H), 4.16 (m, 3H), 4.85 (br s, 1H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.35 (m, 3H), 7.60 (s, 1H), 8.42 (s, 1H)および 10.82 (br s, 1H)

MS (ESI): 464 (MH) $^+$

元素分析	:	実測値	C	66.3	H	6.6	N	12.1
$\text{C}_{26}\text{H}_{30}\text{N}_4\text{O}_4$ 0.5 塩ノール		理論値	C	66.5	H	6.7	N	11.7%

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^1H NMR スペクトル: (DMSO- d_6) 2.10 (s, 3H), 2.20 (s, 3H), 2.40 (m, 10H), 3.98 (s, 3H), 4.13 (m, 3H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.35 (m, 3H), 7.60 (s, 1H), 8.42 (s, 1H)および10.82 (br s, 1H)

MS (ESI): 478 (MH)⁺

元素分析	:	実測値	C 61.6	H 6.4	N 14.4
$\text{C}_{26}\text{H}_{31}\text{N}_5\text{O}_4 \cdot 1.0\text{H}_2\text{O} \cdot 0.25$ 塩ノル		理論値	C 61.6	H 6.8	N 13.9%

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^1H NMR スペクトル: (DMSO- d_6) 2.20 (s, 3H), 2.44 (m, 6H), 3.48 (t, 4H), 3.98 (s, 3H), 4.13 (m, 3H), 4.98 (br s, 1H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.35 (m, 3H), 7.60 (s, 1H), 8.42 (s, 1H)および10.82 (br s, 1H)

MS (ESI): 465 (MH)⁺

元素分析	:	実測値	C 58.5	H 6.0	N 11.2
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_5 \cdot 2.5\text{H}_2\text{O}$		理論値	C 58.9	H 6.5	N 11.0%

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^1H NMR スペクトル: (DMSO- d_6) 2.10 (m, 9H), 2.20 (m, 2H), 3.98 (s, 3H), 4.13 (m, 3H), 4.98 (br s, 1H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.35 (m, 3H), 7.60 (s, 1H), 8.42 (s, 1H) および 10.82 (br s, 1H)

MS (ESI): 423 (MH)⁺

元素分析	:	実測値	C 65.5	H 6.2	N 13.2
$\text{C}_{23}\text{H}_{20}\text{N}_4\text{O}_4$		理論値	C 65.4	H 6.2	N 13.3%

^1H NMR スペクトル: (DMSO- d_6) 0.95 (t, 6H), 2.11 (s, 3H), 2.40 (m, 6H), 3.98 (s, 3H), 4.13 (m, 3H), 4.84 (br s, 1H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.35 (m, 3H), 7.60 (s, 1H), 8.42 (s, 1H)および 10.82 (br s, 1H)

MS (ESI): 451 (MH) $^+$

元素分析	:	実測値	C	64.4	H	6.6	N	12.0
$\text{C}_{25}\text{H}_{30}\text{N}_4\text{O}_4 \cdot 1.0\text{H}_2\text{O}$		理論値	C	64.1	H	6.9	N	12.0%

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^1H NMR スペクトル: (DMSO- d_6) 0.98 (d, 6H), 2.20 (s, 3H), 2.55-2.80 (m, 3H), 3.98 (s, 3H), 4.02-4.20 (m, 3H), 4.98 (br s, 1H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.30-7.40 (m, 3H), 7.60 (s, 1H), 8.42 (s, 1H)および 10.82 (br s, 1H)

MS (ESI): 437 (MH) $^+$

元素分析	:	実測値	C	63.3	H	6.3	N	12.4
$\text{C}_{24}\text{H}_{28}\text{N}_4\text{O}_4 \cdot 1.0\text{H}_2\text{O}$		理論値	C	63.4	H	6.7	N	12.3%

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^1H NMR (DMSO- d_6) 0.98 (d, 12H), 2.20 (s, 3H), 2.72 (m, 2H), 3.00 (m, 2H), 3.98 (s, 3H), 4.11 (m, 3H), 6.98 (dd, 1H), 7.18 (s, 1H), 7.35 (m, 3H), 7.60 (s, 1H), 8.42 (s, 1H)および 10.82 (br s, 1H)

MS (ESI) : 479 (MH) $^+$

元素分析	:	実測値	C	65.4	H	6.8	N	11.3
$\text{C}_{27}\text{H}_{34}\text{N}_4\text{O}_4 \cdot 0.8\text{H}_2\text{O}$		理論値	C	55.8	H	7.2	N	11.4%

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^1H NMR スペクトル: (DMSO- d_6) 1.28 (m, 2H), 2.30 (t, 4H), 2.56 (t, 2H), 2.650 (m, 4H), 3.55 (t, 4H), 3.98 (s, 3H), 4.15 (m, 3H), 6.42 (s, 1H), 6.98 (dd, 1H), 7.42 (m, 4H), 7.60 (s, 1H), 8.45 (s, 1H), および 11.19 (br s, 1H)

MS (ESI) : 508 (MH)⁺

元素分析	:	実測値	C	59.7	H	6.6	N	13.4
$\text{C}_{27}\text{H}_{33}\text{N}_5\text{O}_5 \cdot 1.8\text{H}_2\text{O}$		理論値	C	60.1	H	6.8	N	13.0%

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^1H NMR スペクトル: (DMSO- d_6) 1.55 (m, 2H), 2.10 (s, 3H), 2.30 (t, 8H), 2.62 (m, 6H), 3.98 (s, 3H), 4.12 (m, 3H), 6.42 (s, 1H), 6.98 (dd, 1H), 7.42 (m, 4H), 7.60 (s, 1H), 8.45 (s, 1H), および 11.19 (br s, 1H)

MS (ESI) : 521 (MH)⁺

元素分析	:	実測値	C	61.3	H	7.3	N	16.1
$\text{C}_{28}\text{H}_{36}\text{N}_6\text{O}_4 \cdot 1.6\text{H}_2\text{O}$		理論値	C	61.2	H	7.2	N	16.3%

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¹H NMR スペクトル: (DMSO-d₆) 1.60 (m, 6H), 2.25 (m, 4H), 2.60 (m, 4H), 3.08 (m, 2H), 3.98 (s, 3H), 4.12 (m, 3H), 6.42 (s, 1H), 6.98 (dd, 1H), 7.34 (m, 4H), 7.58 (s, 1H), 8.42 (s, 1H), および 11.80 (br s, 1H)
MS (ESI) : 492 (MH)⁺

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^1H NMR スペクトル: (CDCl_3) 1.47 (m, 2H), 1.60 (m, 4H), 2.14 (m, 2H), 2.44 (m, 4H), 2.54 (t, 2H), 4.08 (s, 3H), 4.27 (t, 2H), 6.67 (m, 1H), 7.15 (d, 1H), 7.32 (t, 1H), 7.36 (s, 1H), 7.42 (d, 1H), 7.69 (s, 1H) 8.55 (br s, 1H) および 8.62 (s, 1H)

MS (ESI): 511, 513 (MH)⁺

元素分析	実測値	C	58.2	H	5.3	N	10.8
$\text{C}_{25}\text{H}_{27}\text{BrN}_4\text{O}_3 \cdot 0.25 \text{H}_2\text{O}$,	理論値	C	58.2	H	5.4	N	10.9%

^1H NMR スペクトル: ($\text{DMSO}-d_6$) 3.83 (s, 3H), 6.90 (d, 1H), 7.16 (d, 1H), 7.40 (d, 1H), 11.88 (br s, 1H) および 13.19 (br s, 1H)

MS (ESI): 268, 270 (M-H)

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MS (ESI): 447 (MH) ⁺							
元素分析	实测值	C	69.5	H	6.8	N	12.5
C ₂₆ H ₃₀ N ₄ O ₃	理論值	C	69.9	H	6.8	N	12.6%

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¹H NMR (CDCl₃): 3.74 (s, 3H), 4.50 (s, 1H), 6.33 (d, 1H), 6.79 (dd, 1H), 7.00 (m, 2H), 7.17 (d, 1H).

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MS (ESI) : 435(MH)⁺

元素分析	実測値	C 63.4	H 5.9	N 12.3
$C_{24}H_{26}N_4O_4 \cdot 1H_2O$	理論値	C 63.7	H 6.2	N 12.4%

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^1H NMR 測定値: (DMSO- d_6) 2.75 (m, 1H), 2.89 (m, 1H), 3.44 (m, 1H), 3.97 (s, 3H), 4.06 (m, 1H), 4.58 (dd, 1H), 6.44 (m, 1H), 6.95 (dd, 1H), 7.40 (m, 4H) 7.62 (s, 1H), 8.47 (s, 1H), 11.19 (br s 1H)

MS (ESI) : 364 (MH) $^+$

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^1H NMR 測定値: (CDCl $_3$) 2.48 (m, 2H), 2.624 (m, 2H), 2.68 (m, 2H), 3.78 (m, 4H), 4.04 (s, 3H), 4.24 (m, 3H), 6.58 (m, 1H), 7.08 (dd, 1H), 7.29 (m, 1H), 7.34 (s, 1H), 7.46 (d, 1H), 7.50 (d, 1H), 7.62 (s, 1H), 8.31 (br s, 1H)および 8.62 (s, 1H)

MS (ESI) : 451(MH) $^+$

元素分析	実測値	C	60.3	H	5.9	N	12.3
C $_{24}$ H $_{26}$ N $_4$ O $_5$ ·1.5H $_2$ O	理論値	C	60.4	H	6.1	N	11.7%

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^1H NMR スペクトル: (CDCl_3) 1.47 (m, 2H), 1.61 (m, 4H), 2.39 (m, 2H), 2.54 (d, 2H), 2.64 (m, 2H), 4.04 (s, 3H), 4.24 (m, 3H), 6.58 (m, 1H), 7.08 (dd, 1H), 7.29 (m, 1H), 7.32 (s, 1H), 7.45 (d, 1H), 7.48 (d, 1H), 7.62 (s, 1H), 8.28 (br s, 1H) および 8.60 (s, 1H)

MS (ESI): 449 (MH)⁺

元素分析	実測値	C	65.9	H	6.3	N	12.3
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_4 \cdot 0.5\text{H}_2\text{O}$	理論値	C	65.6	H	6.4	N	12.3%

^1H NMR スペクトル: (DMSO-d_6) 2.21 (s, 6H), 2.38 (m, 2H), 3.97 (s, 3H), 4.073 (m, 2H), 4.21 (m, 1H), 4.96 (d, 1H), 6.43 (m, 1H), 6.97 (dd, 1H), 7.37 (s, 1H), 7.43 (m, 3H), 7.62 (s, 1H), 8.48 (s, 1H) および 11.20 (br s, 1H)

MS (ESI): 409 (MH)⁺

元素分析	実測値	C	62.8	H	5.8	N	13.2
$\text{C}_{22}\text{H}_{24}\text{N}_4\text{O}_4 \cdot 0.7\text{H}_2\text{O}$	理論値	C	62.8	H	6.1	N	13.3%

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$^1\text{H NMR}$ 測定値: (CDCl_3) 1.08 (m, 12H), 1.57 (m, 1H), 1.75 (m, 1H), 3.10 (m, 2H), 4.04 (s, 3H), 4.16 (m, 3H), 6.58 (m, 1H), 7.08 (dd, 1H), 7.26 (m, 1H), 7.32 (s, 1H), 7.45 (d, 1H), 7.50 (d, 1H), 7.61 (s, 1H), 8.32 (br s, 1H) および 8.61 (s, 1H)

MS (ESI) : 465(MH) $^+$

元素分析	実測値	C	64.8	H	6.8	N	11.9
$\text{C}_{26}\text{H}_{32}\text{N}_4\text{O}_4 \cdot 1.0\text{H}_2\text{O}$	理論値	C	64.6	H	7.0	N	11.6%

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MS (ESI) : 435(MH)⁺

元素分析	実測値	C 64.7	H 6.0	N 12.6
$C_{24}H_{26}N_4O_4 \cdot 0.5H_2O$	理論値	C 64.9	H 6.1	N 12.7%

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^1H NMR スペクトル: (DMSO- d_6) 2.75 (m, 1H), 2.89 (m, 1H), 3.44 (m, 1H), 3.97 (s, 3H), 4.06 (m, 1H), 4.58 (dd, 1H), 6.44 (m, 1H), 6.95 (dd, 1H), 7.46 (m, 4H), 7.62 (s, 1H), 8.47 (s, 1H)および 11.19 (br s 1H)
MS (ESI): 364 (MH)⁺

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^1H NMR スペクトル: (CDCl₃) 2.48 (m, 2H), 2.62 (m, 2H), 2.68 (m, 2H), 3.78 (m, 4H), 4.04 (s, 3H), 4.29 (m, 3H), 6.58 (m, 1H), 7.08 (dd, 1H), 7.29 (m, 1H), 7.34 (s, 1H), 7.46 (d, 1H), 7.50 (d, 1H), 7.62 (s, 1H), 8.31 (br s, 1H)および 8.62 (s, 1H)

MS (ESI): 451(MH)⁺

元素分析	実測値	C	61.7	H	5.7	N	11.8
C ₂₄ H ₂₆ N ₄ O ₅ ·1.0H ₂ O	理論値	C	61.5	H	6.0	N	12.0%

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^1H NMR λ° CDCl_3 : 1.47 (m, 2H), 1.61 (m, 4H), 2.39 (m, 2H), 2.54 (d, 2H), 2.64 (m, 2H), 4.04 (s, 3H), 4.29 (m, 3H), 6.58 (m, 1H), 7.08 (dd, 1H), 7.29 (m, 1H), 7.32 (s, 1H), 7.45 (d, 1H), 7.48 (d, 1H), 7.62 (s, 1H), 8.28 (br s, 1H) および 8.60 (s, 1H)

MS (ESI): 449 (MH)⁺

元素分析	実測値	C	65.8	H	6.2	N	12.2
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_4 \cdot 0.5\text{H}_2\text{O}$	理論値	C	65.6	H	6.4	N	12.3%

^1H NMR λ° DMSO-d_6 : 2.21 (s, 6H), 2.38 (m, 2H), 3.97 (s, 3H), 4.083 (m, 2H), 4.21 (m, 1H), 4.96 (d, 1H), 6.43 (m, 1H), 6.97 (dd, 1H), 7.37 (s, 1H), 7.43 (m, 3H), 7.62 (s, 1H), 8.48 (s, 1H) および 11.20 (br s, 1H)

MS (ESI): 409 (MH)⁺

元素分析	実測値	C	63.6	H	6.0	N	13.3
$\text{C}_{22}\text{H}_{24}\text{N}_4\text{O}_4 \cdot 0.5\text{H}_2\text{O}$	理論値	C	63.3	H	6.0	N	13.4%

^1H NMR λ° CDCl_3 : 1.08 (m, 12H), 1.57 (m, 1H), 1.759 (m, 1H), 3.10 (m, 2H), 4.04 (s, 3H), 4.16 (m, 3H), 6.58 (m, 1H), 7.08 (dd, 1H), 7.26 (m, 1H), 7.32 (s, 1H), 7.45 (d, 1H), 7.50 (d, 1H), 7.61 (s, 1H), 8.32 (br s, 1H) および 8.61 (s, 1H)

MS (ESI) : 465(MH) $^+$

元素分析	実測値	C	67.2	H	7.0	N	11.9
$\text{C}_{26}\text{H}_{32}\text{N}_4\text{O}_4$	理論値	C	67.2	H	6.9	N	12.1%

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^1H NMR スペクトル: (DMSO-d_6) 0.98 (m, 6H), 2.68 (m, 3H), 3.96 (m, 4H), 4.13 (m, 2H), 5.06 (br s, 1H), 6.44 (s, 1H), 6.98 (dd, 1H), 7.439 (m, 4H), 7.60 (s, 1H), 8.46 (s, 1H)および 11.22 (s, 1H)

MS (ESI): 423(MH) $^+$

元素分析	実測値	C	63.6	H	6.4	N	12.9
$\text{C}_{23}\text{H}_{26}\text{N}_4\text{O}_4 \cdot 0.6\text{H}_2\text{O}$	理論値	C	63.8	H	6.3	N	12.9%

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^1H NMR スペクトル: (DMSO-d_6) 0.985 (m, 6H), 2.68 (m, 3H), 3.96 (m, 4H), 4.13 (m, 2H), 5.06 (br s, 1H), 6.44 (s, 1H), 6.98 (dd, 1H), 7.43 (m, 4H), 7.60 (s, 1H), 8.46 (s, 1H)および 11.22 (s, 1H)

MS (ESI): 423(MH) $^+$

元素分析	実測値	C	63.1	H	6.3	N	12.7
$\text{C}_{23}\text{H}_{26}\text{N}_4\text{O}_4 \cdot 0.9\text{H}_2\text{O}$	理論値	C	63.0	H	6.4	N	12.8%

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¹H NMR (λ^o 400 MHz; (DMSO-d₆) 1.60 (s, 4H), 2.38 (s, 3H), 2.57 (m, 6H), 4.11 (m, 6H), 4.95 (d, 1H), 6.14 (s, 1H), 6.88 (dd, 1H), 7.29 (m, 2H), 7.37 (s, 1H), 7.59 (s, 1H), 8.48 (s, 1H)および 11.00 (s, 1H)

MS (ESI) : 450 (MH)⁺

元素分析	実測値	C 67.0	H 6.5	N 12.0
$C_{25}H_{28}N_4O_4 \cdot 0.1 H_2O$	理論値	C 66.7	H 6.3	N 12.4%

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^1H NMR λ° C_6H_6 : (DMSO) 2.40 (s, 3H), 2.75 (m, 1H), 2.90 (m, 1H), 3.40 (m, 1H), 3.98 (s, 3H), 4.05 (m, 1H), 4.60 (m, 1H), 6.15 (s, 1H), 6.85 (dd, 1H), 7.30 (m, 2H) 7.40 (s, 1H), 7.60 (s, 1H), 8.45 (s, 1H)および 10.98 (s, 1H)
MS (ESI) : 378 (MH)⁺

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^1H NMR λ° C_6H_6 : (DMSO) 1.60 (s, 4H), 2.38 (s, 3H), 2.57 (m, 6H), 4.11 (m, 6H), 4.95 (d, 1H), 6.14 (s, 1H), 6.88 (dd, 1H), 7.29 (m, 2H), 7.37 (s, 1H), 7.59 (s, 1H), 8.48 (s, 1H)および 11.00 (s, 1H)
MS (ESI) : 450 (MH)⁺

元素分析	実測値	C	66.8	H	6.3	N	12.4
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_4 \cdot 0.1 \text{H}_2\text{O}$	理論値	C	66.7	H	6.3	N	12.4%

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¹H NMR (λ^o 400 MHz; (DMSO-d₆) 0.99 (d, 6H), 2.39 (s, 3H), 2.66 (m, 3H), 4.07 (m, 6H), 5.08 (d, 1H), 6.14 (s, 1H), 6.88 (dd, 1H), 7.29 (m, 2H), 7.37 (s, 1H), 7.58 (s, 1H), 8.49 (s, 1H)および 11.03 (s, 1H)

MS (ESI) : 437 (MH)⁺

元素分析	実測値	C 64.3	H 6.4	N 12.3
$C_{24}H_{28}N_4O_4 \cdot 0.5 H_2O$	理論値	C 64.7	H 6.6	N 12.6%

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^1H NMR スペクトル: (DMSO-d_6): 0.99 (d, 6H), 2.39 (s, 3H), 2.66 (m, 3H), 4.07 (m, 6H), 5.08 (d, 1H), 6.14 (s, 1H), 6.88 (dd, 1H), 7.29 (m, 2H), 7.37 (s, 1H), 7.58 (s, 1H), 8.49 (s, 1H) および 11.03 (s, 1H)

MS (ESI): 437 (MH)⁺

元素分析	実測値	C	64.3	H	6.5	N	12.3
$\text{C}_{24}\text{H}_{28}\text{N}_4\text{O}_4 \cdot 0.5 \text{H}_2\text{O}$	理論値	C	64.7	H	6.6	N	12.6%

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^1H NMR スペクトル: (CDCl_3) 2.13 (m, 2H), 1.48 (t, 4H), 1.57 (t, 2H), 3.72 (t, 4H), 3.84 (s, 3H), 4.05 (s, 3H), 4.3 (t, 2H), 6.50 (d, 1H), 7.08-7.13 (m, 2H), 7.32 (s, 1H), 7.37 (s, 1H), 7.47 (d, 1H), 7.62 (s, 1H) 8.59 (s, 1H)

MS (ESI): 449 (MH)⁺

元素分析	実測値	C	66.5	H	6.4	N	12.3
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_4 \cdot 0.1 \text{H}_2\text{O}$	理論値	C	66.7	H	6.3	N	12.4%

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^1H NMR λ° CDCl_3) 1.47 (m, 2H), 1.64 (m, 4H), 2.57 (t, 4H) 2.94 (t, 2H), 3.83 (s, 3H), 4.05 (s, 3H), 4.34 (t, 2H), 6.49 (d, 1H), 7.10 (m, 2H), 7.32 (s, 1H), 7.38 (d, 1H), 7.45 (d, 1H), 7.62 (s, 1H) 8.60 (s, 1H)

MS (ESI) : 433 (MH) $^+$

元素分析	実測値	C	69.2	H	6.7	N	12.7
$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_3$	理論値	C	69.4	H	6.5	N	13.0%

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^1H NMR スペクトル: (CDCl_3) 1.81 (m, 4H), 2.18 (m, 2H), 2.56 (m, 4H), 2.69 (t, 2H), 3.82 (s, 3H), 4.05 (s, 3H), 4.30 (t, 2H), 6.45 (d, 1H), 7.09 (dd, 2H), 7.31 (s, 1H), 7.38 (d, 1H), 7.47 (d, 1H), 7.62 (s, 1H) および 8.59 (s, 1H)

MS (ESI): 433 (MH)⁺

元素分析

実測値 C 66.5 H 6.3 N 12.4

$\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_3 \cdot 0.1$ シクロヘキサノール + 0.7 H_2O

理論値 C 66.7 H 6.6 N 12.4%

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^1H NMR スペクトル: (CDCl_3) 1.46 (m, 2H), 1.60 (m, 4H), 2.16 (m, 2H), 2.43 (m, 4H), 2.54 (t, 2H), 3.85 (s, 3H), 4.33 (t, 2H), 7.04 (d, 1H), 7.10 (s, 1H), 7.47 (s, 1H), 7.57 (d, 1H), 7.83 (d, 1H), 7.95 (d, 1H) および 9.09 (s, 1H)

MS (ESI): 478 (MH)⁺

元素分析

実測値 C 62.5 H 5.8 N 14.7

$\text{C}_{25}\text{H}_{27}\text{N}_5\text{O}_3$

理論値 C 62.9 H 5.7 N 14.7%

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^1H NMR スペクトル: ($\text{DMSO}-d_6$) 1.33 (t, 3H), 3.95 (s, 3H), 4.35 (q, 2H), 7.19 (d, 1H), 7.35 (d, 1H), 7.75 (d, 1H) および 12.45 (br s, 1H)

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¹H NMR (CDCl₃) 3.99 (s, 3H), 6.88 (t, 1H), 6.97 (d, 1H), 7.37 (t, 1H), 7.55 (d, 1H) および 8.38 (br s, 1H)
MS (ESI) : 193 (MH)⁺

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¹H NMR 測定条件: (CDCl₃) 6.95 (d, 1H), 7.29 (m, 1H), 7.43 (t, 1H), 7.63 (d, 1H)および11.60 (br s, 1H)
MS (ESI): 177 (M-H)⁻

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^1H NMR スペクトル: (CDCl_3) 1.39(m, 2H), 1.50 (m, 4H), 1.96 (m, 2H), 2.35 (m, 4H), 2.43 (t, 2H), 3.80 (s, 3H), 4.28 (t, 2H), 4.84 (br s, 2H), 6.68 (d, 1H), 6.78 (d, 1H), 6.94 (s, 1H), 7.28 (s, 1H), 7.45 (s, 1H), 7.69 (s, 1H), 8.45 (br s, 1H)および 8.98 (s, 1H)

MS (ESI): 448 (MH)⁺

元素分析

実測値 C 64.0 H 6.4 N 14.4

$\text{C}_{25}\text{H}_{29}\text{N}_5\text{O}_3 \cdot 0.3 \text{H}_2\text{O} + 0.4$ シクロヘキサン

理論値 C 63.6 H 6.3 N 14.4%

^1H NMR スペクトル: (DMSO- d_6) 1.38 (m, 2H), 1.50 (m, 4H), 1.95 (m, 2H), 2.15 (m, 4H), 2.42 (t, 2H), 3.99 (s, 3H), 4.22 (t, 2H), 6.47 (m, 1H), 7.36 (s, 1H), 7.55 (m, 1H), 7.60 (s, 1H), 7.90 (d, 1H), 8.18 (d, 1H), 8.49 (s, 1H) および 11.76 (br s, 1H)

MS (ESI): 434 (MH) $^+$

元素分析	実測値	C	63.9	H	6.4	N	15.4
$\text{C}_{24}\text{H}_{27}\text{N}_5\text{O}_3$ 1.0 H_2O	理論値	C	63.8	H	6.5	N	15.5%

^1H NMR スペクトル: (CDCl_3) 1.48-2.18 (m, 19H), 2.58 (t, 2H), 3.06 (d, 2H), 4.05 (s, 3H), 4.26 (t, 2H), 6.59 (s, 1H), 7.08 (dd, 1H), 7.28 (d, 1H), 7.36 (s, 1H), 7.50 (d, 1H), 7.63 (s, 1H), 8.30 (s, 1H), 8.59 (s, 1H)

MS: 516 [MH] $^+$

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^1H NMR $\lambda^\circ\text{クトル}$: (CDCl_3) 2.46-2.57 (m, 2H), 3.68 (t, 2H), 4.08 (s, 3H),

4.38 (t, 2H), 6.58 (s, 1H), 7.09 (d, 1H), 7.27 (s, 1H), 7.35 (s, 1H), 7.46 (d, 1H),

7.50 (s, 1H), 7.63 (s, 1H), 8.30 (s, 1H), 8.62 (s, 1H)

M S: 428 $[\text{MH}]^+$

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¹H NMR スペクトル: (DMSO-d₆) 1.84-1.96 (m, 1H), 2.10-2.30 (m, 2H), 2.39 (s, 3H), 2.43-2.53 (m, 1H), 2.80 (s, 3H), 3.98 (s, 4H), 4.22 (dd, 1H), 4.40 (dd, 1H), 6.10 (s, 1H), 6.84 (dd, 1H), 7.23 (d, 1H), 7.30 (d, 1H), 7.40 (s, 1H), 7.59 (s, 1H), 8.49 (s, 1H), 10.98 (br s, 1H)

M S: 429 [MH]⁺

元素分析	:	実測値	C	64.4	H	5.4	N	12.6
C ₂₄ H ₂₄ N ₄ O ₄ · 0.8H ₂ O		理論値	C	64.5	H	5.8	N	12.5%

¹H NMR スペクトル: (CDCl₃) 2.10-2.44 (m, 4H), 2.48 (s, 3H), 2.76 (s, 3H), 3.30-3.54 (m, 1H), 4.04 (dd, 1H), 4.15 (dd, 1H), 7.38 (d, 2H), 7.78 (d, 2H)

M S: 284 [MH]⁺

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¹H NMR spectrum (DMSO-d₆) 1.87-2.48 (m, 4H), 3.97 (s, 3H), 4.17 (m, 2H),
6.45 (s, 1H), 6.96 (dd, 1H), 7.38-7.49 (m, 4H), 7.60 (s, 1H), 7.81 (s, 1H), 8.50
(s, 1H)

M S: 405 [MH]⁺

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¹H NMR 測定: (DMSO-d₆) 1.64-2.45 (m, 4H), 3.78 (m, 1H), 3.99 (s, 3H), 4.18 (t, 2H), 6.42 (s, 1H), 6.97 (dd, 1H), 7.38-7.48 (m, 3H), 7.60 (s, 1H), 7.73 (s, 2H), 8.48 (s, 1H), 11.18 (br s, 1H)
MS: 405 [MH]⁺

¹H NMR スペクトル: (CDCl₃) 1.68-1.86 (m, 1H), 2.16-2.38 (m, 3H), 2.48 (s, 3H), 3.86-3.96 (m, 2H), 4.08 (dd, 1H), 6.20 (br s, 1H), 7.38 (d, 2H), 7.80 (d, 2H)
MS: 270 [MH]⁺

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^1H NMR λ° H_2O : (DMSO- d_6) 1.8-2.2 (m, 5H), 2.4 (s, 3H), 4.0 (br s, 3H), 4.1-4.2 (m, 2H), 6.1 (br s, 1H), 6.9 (dd, 1H), 7.2 (d, 1H), 7.3 (d, 1H), 7.4 (s, 1H), 7.6 (s, 1H), 7.8 (s, 1H), 8.5 (s, 1H), 11.0 (br s, 1H)
 MS: 419 [MH] $^+$
 元素分析 : 実測値 C 60.8 H 5.3 N 12.1
 C $_{23}$ H $_{22}$ N $_4$ O $_4$ 2H $_2$ O 理論値 C 60.8 H 5.7 N 12.3%

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^1H NMR スペクトル: (DMSO-d_6) 1.35 (m, 2H), 1.51 (m, 4H), 2.30-2.40 (m, 9H),
 3.98 (s, 3H), 4.08 (m, 2H), 4.21 (m, 1H), 4.86 (m, 1H), 6.10 (s, 1H), 6.87
 (dd, 1H), 7.25 (d, 1H) 7.30 (d, 1H), 7.40 (s, 1H), 7.60 (s, 1H), 8.45 (s, 1H)およ
 び 10.98 (br s, 1H)

MS (ESI) : 463 (MH)⁺

元素分析	:	実測値	C	66.5	H	6.6	N	12.0
$\text{C}_{26}\text{H}_{30}\text{N}_4\text{O}_4 \cdot 0.4\text{H}_2\text{O}$		理論値	C	66.5	H	6.6	N	11.9%

^1H NMR スペクトル: (DMSO-d_6) 1.35 (m, 2H), 1.51 (m, 4H), 2.30-2.40 (m, 9H), 3.98 (s, 3H), 4.08 (m, 2H), 4.21 (m, 1H), 4.86 (m, 1H), 6.10 (s, 1H), 6.87 (dd, 1H), 7.25 (d, 1H), 7.30 (d, 1H), 7.40 (s, 1H), 7.60 (s, 1H), 8.45 (s, 1H) および 10.98 (br s, 1H)

MS (ESI): 463 (MH)⁺

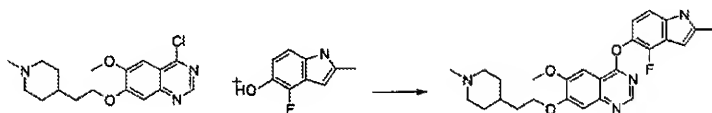
元素分析	:	実測値	C 66.2	H 6.8	N 11.9
$\text{C}_{26}\text{H}_{30}\text{N}_4\text{O}_4 \cdot 0.5\text{H}_2\text{O}$		理論値	C 66.2	H 6.6	N 11.9%

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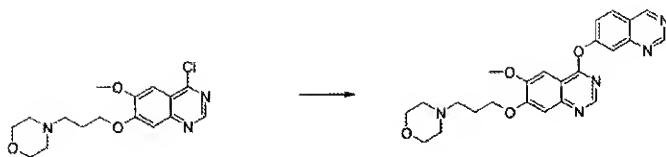
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MS-ESI: 465 [MH]⁺

¹H NMR λ° η η : (DMSO-d₆) 1.1-1.3 (m, 2H); 1.35-1.5 (m, 1H); 1.6-1.9 (m, 6H); 2.12 (s, 3H); 2.4 (s, 3H); 2.75 (d, 2H); 3.95 (s, 3H); 4.22 (t, 2H); 6.2 (s, 1H); 6.95 (dd, 1H); 7.15 (d, 1H); 7.4 (s, 1H); 7.6 (s, 1H); 8.5 (s, 1H)

¹H NMR λ° η η : (DMSO-d₆) 2.50 (s, 3H); 3.95 (s, 3H); 4.0 (s, 3H); 7.05 (d, 1H); 7.38 (s, 1H); 7.39 (d, 1H); 7.51 (d, 1H); 7.60 (s, 1H); 8.50 (s, 1H)

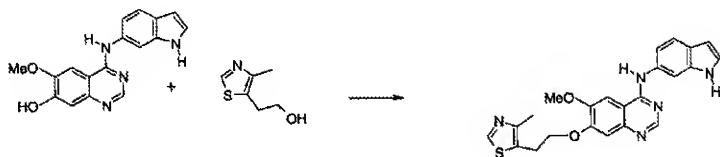
MS (ESI): 337 [MH]⁺



$^1\text{H NMR}$ λ° H_2O (DMSO- d_6) 2.01 (t, 2H); 2.47 (m, 4H); 2.49 (m, 2H); 3.60 (m, 4H); 4.01 (s, 3H); 4.29 (t, 2H); 7.45 (s, 1H); 7.65 (s, 1H); 7.80 (d, 1H); 8.01 (d, 1H); 8.32 (d, 1H); 8.60 (s, 1H); 9.34 (s, 1H); 9.69 (s, 1H)

MS (ESI): 448 [MH] $^+$

元素分析	:	実測値	C	63.4	H	5.7	N	15.6
$\text{C}_{24}\text{H}_{25}\text{N}_5\text{O}_4 \cdot 0.4 \text{H}_2\text{O}$		理論値	C	63.4	H	5.7	N	15.4%



MS - ESI : 432 [MH]⁺

¹H NMR (CDCl₃) : 2.4 (s, 3H) ; 3.3 (t, 2H) ; 4.0 (s, 3H) ; 4.35 (t, 2H) ; 6.45 (s, 1H) ; 7.2 (s, 1H) ; 7.25-7.4 (m, 2H) ; 7.55 (d, 1H) ; 7.9 (s, 1H) ; 8.05 (s, 1H) ; 8.45 (s, 1H) ; 8.87 (s, 1H) ; 9.45 (s, 1H)

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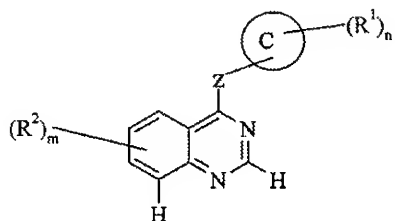
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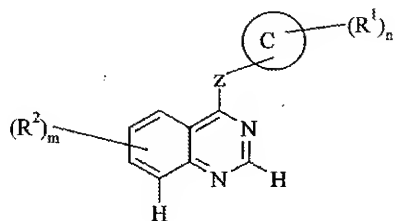
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..... $\partial_{x_1} u$ $\nabla u \cdot \nabla^2 u$ ∇u $\partial_{x_1} u$

..... $\nabla^2 u$ $\nabla^2 u$ $\partial_{x_1} u \cdot \nabla^2 u$

..... $\nabla^2 u$ $\partial_{x_1} u$ $\nabla^2 u$ $\nabla^2 u$ $\nabla^2 u$

..... $\nabla^2 u$ $\partial_{x_1} u$ $\partial_{x_2} u$ $\partial_{x_3} u$

..... $\nabla^2 u$ $\partial_{x_1} u$

.....

..... $\partial_{x_1} u$

..... $\partial_{x_1} u$

..... $\partial_{x_1} u$ $\partial_{x_2} u$

.....

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..... $\partial_{x_1} u$ $\nabla u \cdot \partial_{x_1} u$ $\nabla u \cdot \nabla^2 u$ ∇u ∇u

[illegible]

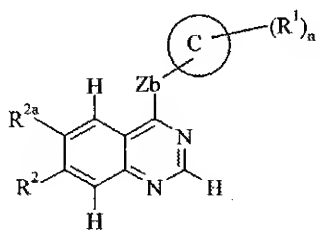
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(II)

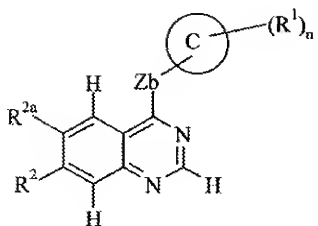
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[illegible]

[illegible]

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(IIb)

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..... V_{11}, V_{12}, \dots V_{11}^* $V_{12}^* \dots \dots \dots$ P_{11}, P_{12}, \dots P_{11}, P_{12}, \dots

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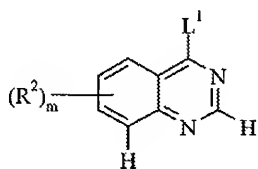
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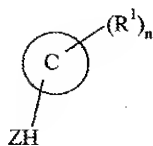
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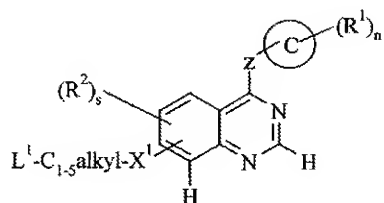
(III)



(IV)

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[illegible]



(IX)

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INTERNATIONAL SEARCH REPORT

International Application No.
P./68 08/06373

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 A61K31/505 C07D401/14 C07D413/14 C07B417/12 C07D405/12
C07D401/12

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS RESEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 A61K C07D

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched:

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 96 29301 A (AGREVO UK LTD ; CORNELL CLIVE LEONARD (GB); RICHARDS IAN CHRISTOPHE) 26 September 1996 (1996-09-26) see compounds 67 and 83 ---	9-11, 14
X	WO 95 15758 A (HSU CHIN YI JENNY ; ZILBERSTEIN ASHER (US); JOHNSON SUSAN E (US); M) 15 June 1995 (1995-06-15) see compound on top of page 17 the whole document ---	9-11, 14, 19-21
Y	---	1-22
	--- -/-	

☒ Further documents are listed in the conclusion of two C.

☒ Patent family members are listed in annex.

* Special categorization of cited documents:

- *A* document defining the general state of the art which is not considered to be of particular relevance
- *B* earlier document but published on or after the international filing date
- *L* document which may form double or priority claim(s) or which is cited to establish the publication date of another document or other special reason (see paragraph 2)
- *O* document referring to an oral disclosure, use, exhibition or other means
- *P* document published prior to the international filing date but later than the priority date claimed

- *** later document published after the international filing date or priority date and not in conflict with the application but which is considered the principle or theory underlying the invention
- ** document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
- ** document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is considered with one or more other such documents, such combination being obvious to a person skilled in the art.
- *E* document member of the same patent family

Date of the actual completion of the international search

7 April 2000

Date of mailing of the international search report

18.05.00

Name and mailing address of the ISA
European Patent Office, P.O. Box 29116 Patenthaus 2
D-60029 Frankfurt am Main
Tel: (+31-70) 340-2040, Tx: 51851 apo nl,
Fax: (+31-70) 340-3016

Authorized officer

Scruton-Evans, I

INTERNATIONAL SEARCH REPORT

Int. Patent Application No.

P-1/GE 00/00373

A. (Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Reason of document, with indicators, where appropriate, of the relevant passages	Relevant to claim No.
P, Y	HENNEQUIN L F ET AL: "Design and Structure-Activity Relationship of a New Class of Potent VEGF Receptor Tyrosine Kinase Inhibitors" J. MED. CHEM. (JMCHEM, 00222623); 1999; VOL. 42 (26); PP. 5369-5389, XP003197180 AstraZeneca Zeneca Pharma Centre de Recherches Z.I. La Pompelle; Reims; 51689; Fr. (FR) the whole document	1-22
Y	BRIDGES A J ET AL: "Enantioselective inhibition of the epidermal growth factor receptor tyrosine kinase by 4-[(alpha-phenethylamino)quinazolines" BIOORG. MED. CHEM. (BMECEP, 09680896); 1995; VOL. 3 (12); PP. 1651-6, XP002134974 Parke-Davis Pharmaceutical Research Division; Ann Arbor; 48105; MI; USA (US) the whole document	1-22
Y	GIBSON K H ET AL: "Epidermal growth factor receptor tyrosine kinase: structure-activity relationships and antitumor activity of novel quinazolines" BIOORG. MED. CHEM. LETT. (BMCLEB, 0960894K); 1997; VOL. 7 (21); PP. 2723-2728, XP002134975 Zeneca Pharmaceuticals; Research Dep. Cancer, Metabolism and Endocrine; Alderley Park, Macclesfield, Cheshire; SK10 4TG; UK (GB) the whole document	1-22
Y	EP 0 602 851 A (ZENECA LTD) 22 June 1994 (1994-06-22) the whole document	1-22
X	WO 97 42187 A (LOHMANN JEAN JACQUES MARCEL ; PLE PATRICK (FR); HENNEQUIN LAURENT F) 13 November 1997 (1997-11-13) see the general formula I and pages 1-3	1-3, 6-8, 20
P, X	WO 99 10349 A (LOHMANN JEAN JACQUES MARCEL ; PLE PATRICK (FR); HENNEQUIN LAURENT F) 4 March 1999 (1999-03-04) the whole document	1-3, 5-8, 20
Y	WO 97 22596 A (ZENECA LTD ; ZENECA PHARMA SA (FR); LOHMANN JEAN JACQUES MARCEL (FR) 26 June 1997 (1997-06-26) the whole document	1-22

INTERNATIONAL SEARCH REPORT

International application No.
PCT/GB 00/00373**Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)**

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☒ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:
Although claim 22 is directed to a method of treatment of the human/animal body, the search has been carried out and based on the alleged effects of the compound
2. ☐ Claims Nos.:
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of Item 2 of first sheet)

This International Searching Authority found multiple inventions in the international application, as follows:

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest.
- ☐ No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No.

PCT/GB 00/00373

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
WO 9629301 A	26-09-1996	AU 5116096 A EP 0819111 A JP 11503114 T ZA 9602319 A	08-10-1996 21-01-1998 23-03-1999 30-10-1996
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